



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:58 PM UTC

PDB ID : 5W9K / pdb_00005w9k
EMDB ID : EMD-8786
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

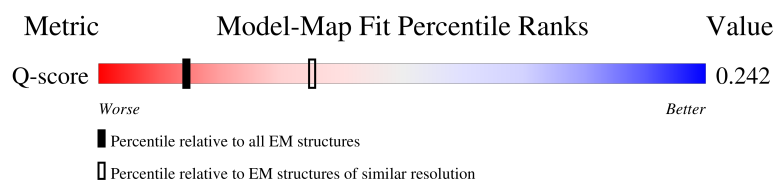
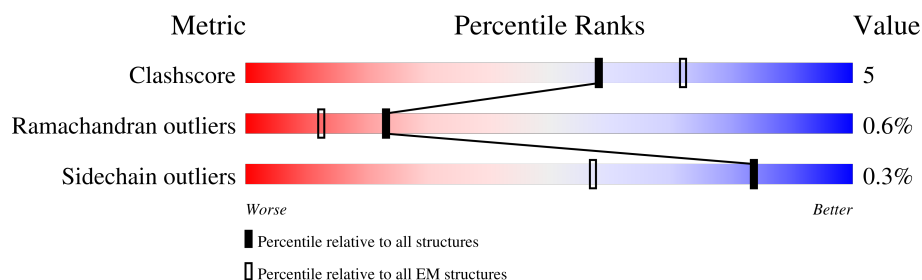
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1329	
1	D	1329	
1	G	1329	
1	J	1329	

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Mol	Chain	Length	Quality of chain
1	K	1329	
1	L	1329	
2	B	233	
2	E	233	
2	H	233	
3	C	218	
3	F	218	
3	I	218	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32873 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	461	Total	C	N	O	S	0	0
			3531	2233	598	683	17		
1	D	462	Total	C	N	O	S	0	0
			3538	2238	599	684	17		
1	G	460	Total	C	N	O	S	0	0
			3527	2231	597	682	17		
1	J	724	Total	C	N	O	S	0	0
			5645	3593	924	1094	34		
1	K	724	Total	C	N	O	S	0	0
			5645	3593	924	1094	34		
1	L	723	Total	C	N	O	S	0	0
			5638	3589	923	1092	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	conflict	UNP W5ZZF5
A	1061	PRO	LEU	conflict	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	conflict	UNP W5ZZF5
D	1061	PRO	LEU	conflict	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	conflict	UNP W5ZZF5
G	1061	PRO	LEU	conflict	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	conflict	UNP W5ZZF5
J	1061	PRO	LEU	conflict	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
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J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5
K	506	PHE	LEU	conflict	UNP W5ZZF5
K	748	ALA	ARG	conflict	UNP W5ZZF5
K	751	GLY	ARG	conflict	UNP W5ZZF5
K	1060	PRO	VAL	conflict	UNP W5ZZF5
K	1061	PRO	LEU	conflict	UNP W5ZZF5
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K	1293	SER	-	expression tag	UNP W5ZZF5
K	1294	GLY	-	expression tag	UNP W5ZZF5
K	1295	TYR	-	expression tag	UNP W5ZZF5
K	1296	ILE	-	expression tag	UNP W5ZZF5
K	1297	PRO	-	expression tag	UNP W5ZZF5
K	1298	GLU	-	expression tag	UNP W5ZZF5
K	1299	ALA	-	expression tag	UNP W5ZZF5
K	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1301	ARG	-	expression tag	UNP W5ZZF5
K	1302	ASP	-	expression tag	UNP W5ZZF5
K	1303	GLY	-	expression tag	UNP W5ZZF5
K	1304	GLN	-	expression tag	UNP W5ZZF5
K	1305	ALA	-	expression tag	UNP W5ZZF5
K	1306	TYR	-	expression tag	UNP W5ZZF5
K	1307	VAL	-	expression tag	UNP W5ZZF5
K	1308	ARG	-	expression tag	UNP W5ZZF5
K	1309	LYS	-	expression tag	UNP W5ZZF5
K	1310	ASP	-	expression tag	UNP W5ZZF5
K	1311	GLY	-	expression tag	UNP W5ZZF5
K	1312	GLU	-	expression tag	UNP W5ZZF5
K	1313	TRP	-	expression tag	UNP W5ZZF5
K	1314	VAL	-	expression tag	UNP W5ZZF5
K	1315	LEU	-	expression tag	UNP W5ZZF5
K	1316	LEU	-	expression tag	UNP W5ZZF5
K	1317	SER	-	expression tag	UNP W5ZZF5
K	1318	THR	-	expression tag	UNP W5ZZF5
K	1319	PHE	-	expression tag	UNP W5ZZF5
K	1320	LEU	-	expression tag	UNP W5ZZF5
K	1321	GLY	-	expression tag	UNP W5ZZF5
K	1322	ARG	-	expression tag	UNP W5ZZF5
K	1323	SER	-	expression tag	UNP W5ZZF5
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K	1325	GLU	-	expression tag	UNP W5ZZF5
K	1326	VAL	-	expression tag	UNP W5ZZF5
K	1327	LEU	-	expression tag	UNP W5ZZF5
K	1328	PHE	-	expression tag	UNP W5ZZF5
K	1329	GLN	-	expression tag	UNP W5ZZF5
L	506	PHE	LEU	conflict	UNP W5ZZF5
L	748	ALA	ARG	conflict	UNP W5ZZF5
L	751	GLY	ARG	conflict	UNP W5ZZF5
L	1060	PRO	VAL	conflict	UNP W5ZZF5
L	1061	PRO	LEU	conflict	UNP W5ZZF5
L	1292	GLY	-	expression tag	UNP W5ZZF5
L	1293	SER	-	expression tag	UNP W5ZZF5
L	1294	GLY	-	expression tag	UNP W5ZZF5
L	1295	TYR	-	expression tag	UNP W5ZZF5
L	1296	ILE	-	expression tag	UNP W5ZZF5
L	1297	PRO	-	expression tag	UNP W5ZZF5
L	1298	GLU	-	expression tag	UNP W5ZZF5
L	1299	ALA	-	expression tag	UNP W5ZZF5

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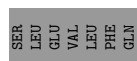
Chain	Residue	Modelled	Actual	Comment	Reference
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L	1302	ASP	-	expression tag	UNP W5ZZF5
L	1303	GLY	-	expression tag	UNP W5ZZF5
L	1304	GLN	-	expression tag	UNP W5ZZF5
L	1305	ALA	-	expression tag	UNP W5ZZF5
L	1306	TYR	-	expression tag	UNP W5ZZF5
L	1307	VAL	-	expression tag	UNP W5ZZF5
L	1308	ARG	-	expression tag	UNP W5ZZF5
L	1309	LYS	-	expression tag	UNP W5ZZF5
L	1310	ASP	-	expression tag	UNP W5ZZF5
L	1311	GLY	-	expression tag	UNP W5ZZF5
L	1312	GLU	-	expression tag	UNP W5ZZF5
L	1313	TRP	-	expression tag	UNP W5ZZF5
L	1314	VAL	-	expression tag	UNP W5ZZF5
L	1315	LEU	-	expression tag	UNP W5ZZF5
L	1316	LEU	-	expression tag	UNP W5ZZF5
L	1317	SER	-	expression tag	UNP W5ZZF5
L	1318	THR	-	expression tag	UNP W5ZZF5
L	1319	PHE	-	expression tag	UNP W5ZZF5
L	1320	LEU	-	expression tag	UNP W5ZZF5
L	1321	GLY	-	expression tag	UNP W5ZZF5
L	1322	ARG	-	expression tag	UNP W5ZZF5
L	1323	SER	-	expression tag	UNP W5ZZF5
L	1324	LEU	-	expression tag	UNP W5ZZF5
L	1325	GLU	-	expression tag	UNP W5ZZF5
L	1326	VAL	-	expression tag	UNP W5ZZF5
L	1327	LEU	-	expression tag	UNP W5ZZF5
L	1328	PHE	-	expression tag	UNP W5ZZF5
L	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

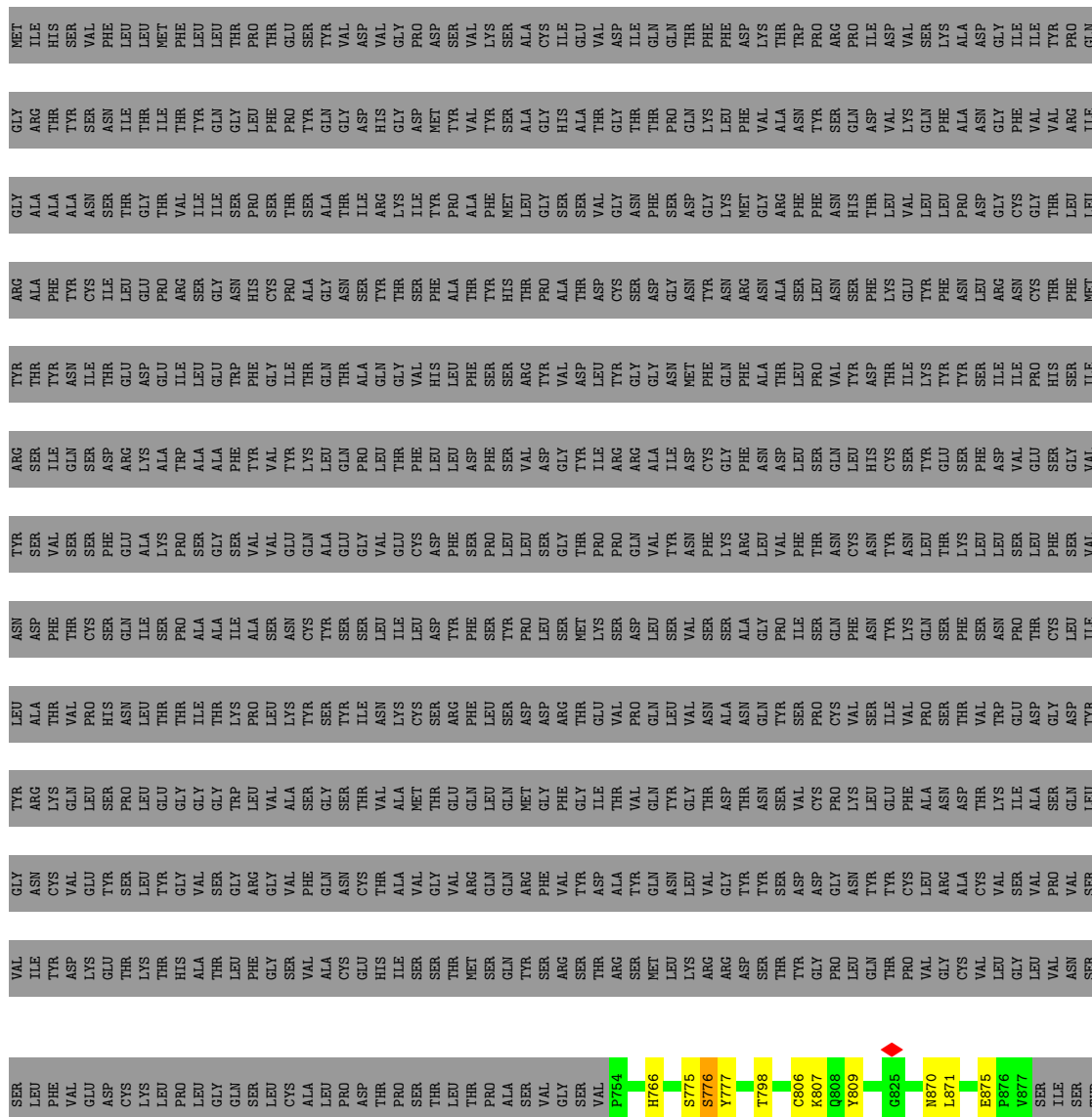
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

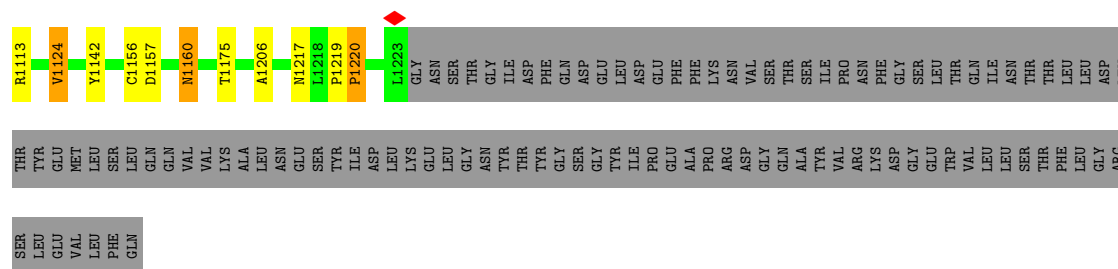
- Molecule 3 is a protein called G4 VL.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

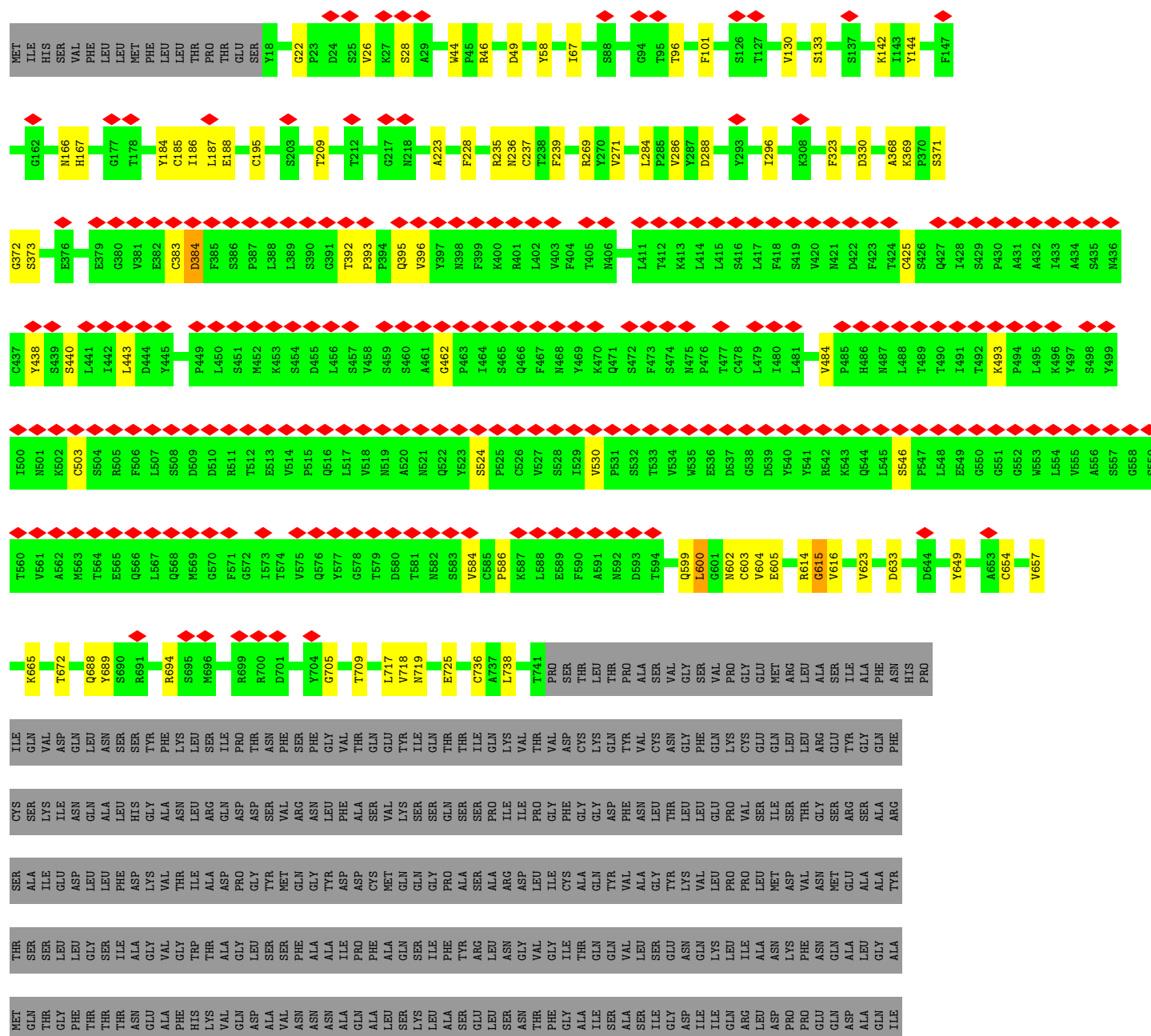


Chain D: 32% 65%





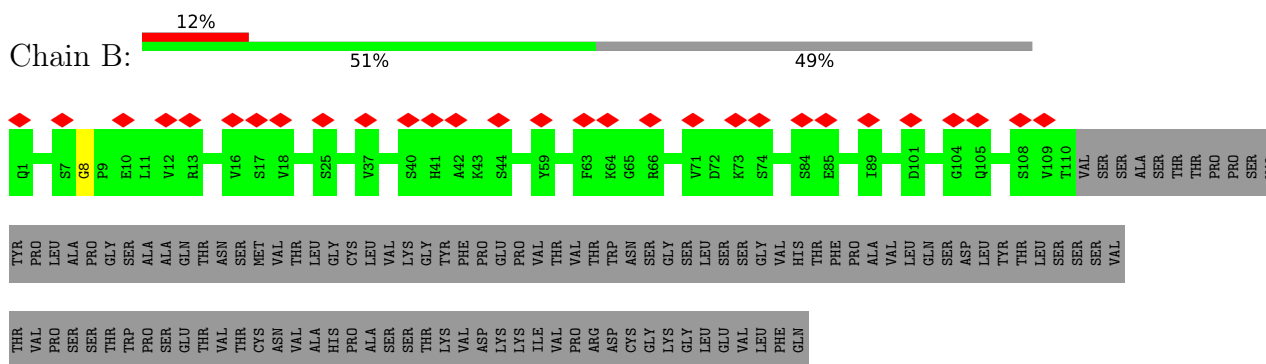
• Molecule 1: Spike glycoprotein



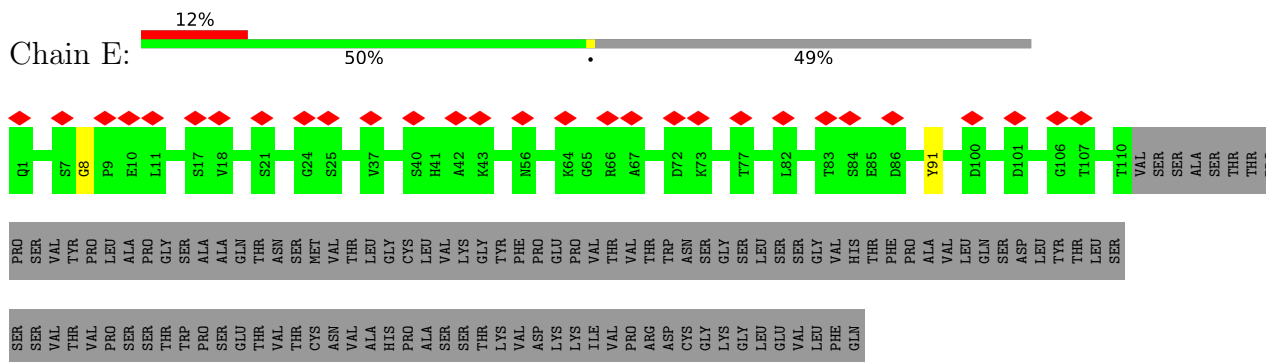


[illegible]

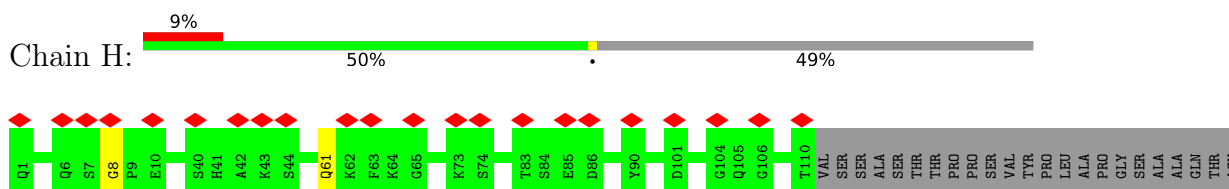
- Molecule 2: G4 VH

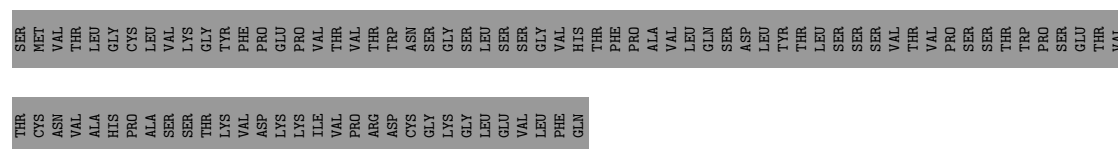


- Molecule 2: G4 VH

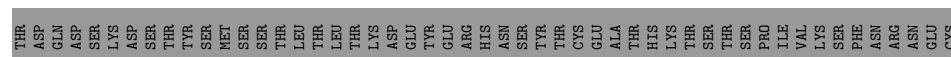
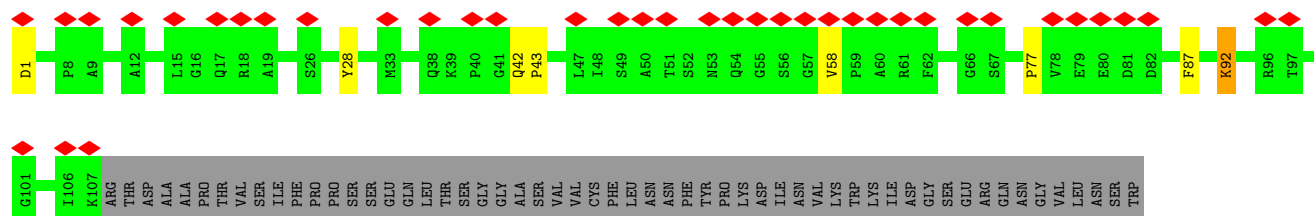


- Molecule 2: G4 VH

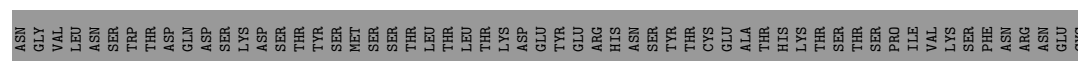
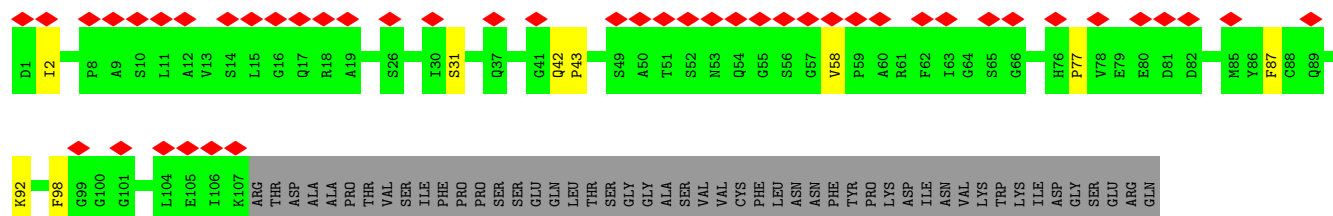




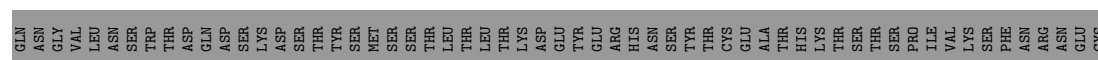
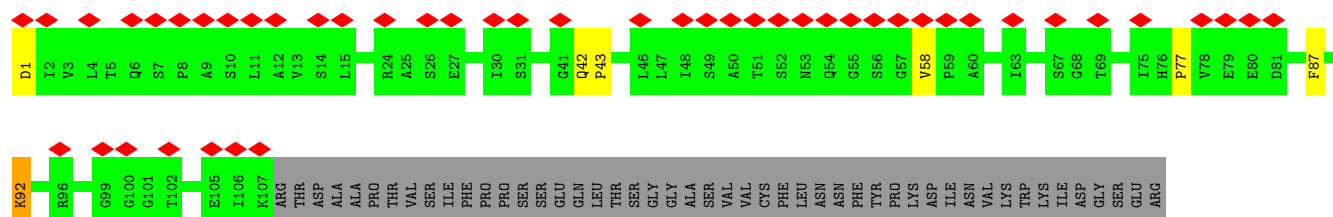
• Molecule 3: G4 VL



• Molecule 3: G4 VL



• Molecule 3: G4 VL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10544	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.90	0/3603	1.24	33/4899 (0.7%)
1	D	0.89	1/3611 (0.0%)	1.23	35/4910 (0.7%)
1	G	0.92	0/3599	1.25	37/4894 (0.8%)
1	J	0.84	3/5789 (0.1%)	1.35	82/7881 (1.0%)
1	K	0.86	8/5789 (0.1%)	1.36	87/7881 (1.1%)
1	L	0.83	3/5782 (0.1%)	1.36	86/7871 (1.1%)
2	B	0.76	0/972	1.12	2/1317 (0.2%)
2	E	0.78	0/972	1.17	3/1317 (0.2%)
2	H	0.75	0/972	1.12	2/1317 (0.2%)
3	C	0.77	0/852	1.33	8/1153 (0.7%)
3	F	0.84	0/852	1.43	10/1153 (0.9%)
3	I	0.78	0/852	1.34	9/1153 (0.8%)
All	All	0.86	15/33645 (0.0%)	1.30	394/45746 (0.9%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	186	ILE	N-CA	8.21	1.56	1.46
1	J	425	CYS	CA-C	-7.72	1.43	1.52
1	K	185	CYS	CA-C	7.60	1.62	1.52
1	K	437	CYS	C-N	7.37	1.43	1.33
1	L	236	ASN	C-N	6.00	1.41	1.33
1	K	437	CYS	N-CA	5.90	1.53	1.46
1	J	383	CYS	CA-CB	5.77	1.61	1.53
1	K	425	CYS	C-N	5.53	1.42	1.33
1	K	608	LEU	CA-C	-5.44	1.46	1.52
1	K	425	CYS	CA-C	-5.43	1.45	1.52
1	J	425	CYS	C-N	5.28	1.40	1.33
1	D	1219	PRO	CA-C	5.24	1.57	1.52
1	K	424	THR	CA-C	-5.19	1.46	1.52
1	K	236	ASN	C-N	5.17	1.40	1.33
1	L	736	CYS	CA-C	5.17	1.59	1.52

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	736	CYS	N-CA-C	-11.87	91.27	108.96
1	L	185	CYS	O-C-N	-10.53	110.99	123.10
3	C	42	GLN	CA-C-N	10.16	126.97	119.66
3	C	42	GLN	C-N-CA	10.16	126.97	119.66
3	I	58	VAL	CA-C-N	9.94	130.56	119.92
3	I	58	VAL	C-N-CA	9.94	130.56	119.92
3	C	58	VAL	CA-C-N	9.89	130.50	119.92
3	C	58	VAL	C-N-CA	9.89	130.50	119.92
1	J	144	TYR	CA-C-N	9.87	129.82	119.85
1	J	144	TYR	C-N-CA	9.87	129.82	119.85
3	F	98	PHE	CA-CB-CG	9.82	123.62	113.80
3	I	42	GLN	CA-C-N	9.77	126.69	119.66
3	I	42	GLN	C-N-CA	9.77	126.69	119.66
3	F	42	GLN	CA-C-N	9.65	126.70	119.66
3	F	42	GLN	C-N-CA	9.65	126.70	119.66
1	K	284	LEU	CA-C-N	9.51	129.16	119.56
1	K	284	LEU	C-N-CA	9.51	129.16	119.56
1	L	735	LEU	CA-C-N	-9.45	106.37	121.87
1	L	735	LEU	C-N-CA	-9.45	106.37	121.87
1	K	144	TYR	CA-C-N	9.43	129.37	119.85
1	K	144	TYR	C-N-CA	9.43	129.37	119.85
1	J	101	PHE	CA-CB-CG	9.38	123.18	113.80
2	E	8	GLY	CA-C-N	9.30	129.25	119.85
2	E	8	GLY	C-N-CA	9.30	129.25	119.85
1	D	935	LEU	CA-C-N	9.09	126.20	119.66
1	D	935	LEU	C-N-CA	9.09	126.20	119.66
1	J	462	GLY	CA-C-N	8.96	128.70	119.56
1	J	462	GLY	C-N-CA	8.96	128.70	119.56
1	J	369	LYS	CA-C-N	8.88	128.82	120.03
1	J	369	LYS	C-N-CA	8.88	128.82	120.03
1	L	462	GLY	CA-C-N	8.86	128.60	119.56
1	L	462	GLY	C-N-CA	8.86	128.60	119.56
1	L	284	LEU	CA-C-N	8.74	128.47	119.56
1	L	284	LEU	C-N-CA	8.74	128.47	119.56
3	F	58	VAL	CA-C-N	8.68	128.63	120.03
3	F	58	VAL	C-N-CA	8.68	128.63	120.03
1	L	393	PRO	CA-C-N	8.65	128.59	120.03
1	L	393	PRO	C-N-CA	8.65	128.59	120.03
1	G	935	LEU	CA-C-N	8.65	125.89	119.66
1	G	935	LEU	C-N-CA	8.65	125.89	119.66
1	J	284	LEU	CA-C-N	8.64	128.37	119.56
1	J	284	LEU	C-N-CA	8.64	128.37	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	935	LEU	CA-C-N	8.63	125.88	119.66
1	A	935	LEU	C-N-CA	8.63	125.88	119.66
1	L	209	THR	CA-C-N	8.49	128.22	119.56
1	L	209	THR	C-N-CA	8.49	128.22	119.56
1	K	185	CYS	CA-C-O	-8.48	112.37	121.45
1	K	393	PRO	CA-C-N	8.47	128.42	120.03
1	K	393	PRO	C-N-CA	8.47	128.42	120.03
1	K	373	SER	N-CA-C	8.44	121.82	110.35
1	L	369	LYS	CA-C-N	8.43	128.37	120.03
1	L	369	LYS	C-N-CA	8.43	128.37	120.03
1	J	209	THR	CA-C-N	8.42	128.14	119.56
1	J	209	THR	C-N-CA	8.42	128.14	119.56
1	L	144	TYR	CA-C-N	8.31	128.25	119.85
1	L	144	TYR	C-N-CA	8.31	128.25	119.85
2	H	8	GLY	CA-C-N	8.30	128.23	119.85
2	H	8	GLY	C-N-CA	8.30	128.23	119.85
1	D	902	ASP	CA-C-N	8.29	128.22	119.85
1	D	902	ASP	C-N-CA	8.29	128.22	119.85
1	G	1219	PRO	CA-C-N	8.20	128.83	120.38
1	G	1219	PRO	C-N-CA	8.20	128.83	120.38
1	K	493	LYS	CA-C-N	8.19	128.12	119.85
1	K	493	LYS	C-N-CA	8.19	128.12	119.85
1	K	133	SER	CA-C-N	8.16	127.88	119.56
1	K	133	SER	C-N-CA	8.16	127.88	119.56
1	K	209	THR	CA-C-N	8.16	127.88	119.56
1	K	209	THR	C-N-CA	8.16	127.88	119.56
1	G	902	ASP	CA-C-N	8.14	128.16	119.78
1	G	902	ASP	C-N-CA	8.14	128.16	119.78
1	L	738	LEU	CA-C-N	8.03	127.95	119.85
1	L	738	LEU	C-N-CA	8.03	127.95	119.85
1	J	530	VAL	CA-C-N	8.01	128.49	119.92
1	J	530	VAL	C-N-CA	8.01	128.49	119.92
1	A	912	CYS	CA-C-N	8.01	132.84	120.75
1	A	912	CYS	C-N-CA	8.01	132.84	120.75
1	J	484	VAL	CA-C-N	8.00	128.02	119.78
1	J	484	VAL	C-N-CA	8.00	128.02	119.78
1	K	96	THR	CA-C-N	8.00	128.02	119.78
1	K	96	THR	C-N-CA	8.00	128.02	119.78
1	K	462	GLY	CA-C-N	7.96	127.68	119.56
1	K	462	GLY	C-N-CA	7.96	127.68	119.56
1	K	185	CYS	O-C-N	7.94	132.23	123.10
1	D	1219	PRO	CA-C-N	7.93	128.55	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1219	PRO	C-N-CA	7.93	128.55	120.38
1	J	738	LEU	CA-C-N	7.92	127.85	119.85
1	J	738	LEU	C-N-CA	7.92	127.85	119.85
1	J	393	PRO	CA-C-N	7.87	127.80	119.85
1	J	393	PRO	C-N-CA	7.87	127.80	119.85
1	A	1219	PRO	CA-C-N	7.86	128.47	120.38
1	A	1219	PRO	C-N-CA	7.86	128.47	120.38
3	F	43	PRO	CA-C-N	7.84	127.77	119.85
3	F	43	PRO	C-N-CA	7.84	127.77	119.85
1	L	530	VAL	CA-C-N	7.82	128.28	119.92
1	L	530	VAL	C-N-CA	7.82	128.28	119.92
1	A	902	ASP	CA-C-N	7.80	127.82	119.78
1	A	902	ASP	C-N-CA	7.80	127.82	119.78
1	J	383	CYS	CA-C-O	7.79	129.62	120.58
1	L	185	CYS	CA-C-O	7.77	129.76	121.45
1	L	493	LYS	CA-C-N	7.75	127.67	119.85
1	L	493	LYS	C-N-CA	7.75	127.67	119.85
1	J	133	SER	CA-C-N	7.72	127.44	119.56
1	J	133	SER	C-N-CA	7.72	127.44	119.56
1	J	493	LYS	CA-C-N	7.66	127.59	119.85
1	J	493	LYS	C-N-CA	7.66	127.59	119.85
1	D	1142	TYR	CA-C-N	7.58	127.59	119.78
1	D	1142	TYR	C-N-CA	7.58	127.59	119.78
1	K	236	ASN	CA-C-N	-7.56	110.61	121.42
1	K	236	ASN	C-N-CA	-7.56	110.61	121.42
1	L	484	VAL	CA-C-N	7.55	127.56	119.78
1	L	484	VAL	C-N-CA	7.55	127.56	119.78
1	L	133	SER	CA-C-N	7.54	127.25	119.56
1	L	133	SER	C-N-CA	7.54	127.25	119.56
1	K	378	ALA	CA-C-N	7.51	135.21	121.70
1	K	378	ALA	C-N-CA	7.51	135.21	121.70
1	L	96	THR	CA-C-N	7.50	127.50	119.78
1	L	96	THR	C-N-CA	7.50	127.50	119.78
1	K	530	VAL	CA-C-N	7.41	127.42	119.78
1	K	530	VAL	C-N-CA	7.41	127.42	119.78
1	J	717	LEU	N-CA-C	7.40	120.41	111.82
1	G	1142	TYR	CA-C-N	7.37	127.37	119.78
1	G	1142	TYR	C-N-CA	7.37	127.37	119.78
1	J	22	GLY	CA-C-N	7.33	127.33	119.78
1	J	22	GLY	C-N-CA	7.33	127.33	119.78
1	J	688	GLN	N-CA-C	7.31	120.67	111.24
1	A	1142	TYR	CA-C-N	7.22	127.21	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1142	TYR	C-N-CA	7.22	127.21	119.78
2	B	8	GLY	CA-C-N	7.20	127.20	119.78
2	B	8	GLY	C-N-CA	7.20	127.20	119.78
1	J	425	CYS	CA-C-O	-7.05	113.90	121.45
1	J	96	THR	CA-C-N	7.03	127.02	119.78
1	J	96	THR	C-N-CA	7.03	127.02	119.78
3	I	58	VAL	N-CA-C	7.01	116.86	108.45
3	F	58	VAL	N-CA-C	7.00	116.85	108.45
1	L	717	LEU	N-CA-C	6.99	119.93	111.82
1	K	649	TYR	CA-C-N	-6.97	113.17	122.99
1	K	649	TYR	C-N-CA	-6.97	113.17	122.99
1	J	705	GLY	CA-C-N	6.91	126.90	119.78
1	J	705	GLY	C-N-CA	6.91	126.90	119.78
1	J	688	GLN	CA-C-N	6.89	134.10	121.70
1	J	688	GLN	C-N-CA	6.89	134.10	121.70
1	D	1219	PRO	N-CA-C	6.88	119.10	110.70
1	K	392	THR	CA-C-N	6.87	124.61	119.66
1	K	392	THR	C-N-CA	6.87	124.61	119.66
1	D	1160	ASN	CA-C-N	6.87	128.42	119.84
1	D	1160	ASN	C-N-CA	6.87	128.42	119.84
1	L	269	ARG	N-CA-C	6.86	118.76	111.28
1	J	188	GLU	CA-C-N	6.86	126.78	119.85
1	J	188	GLU	C-N-CA	6.86	126.78	119.85
1	L	223	ALA	N-CA-C	6.85	118.40	111.07
1	A	1220	PRO	N-CA-C	6.81	119.01	110.70
3	C	43	PRO	CA-C-N	6.77	126.69	119.85
3	C	43	PRO	C-N-CA	6.77	126.69	119.85
1	A	766	HIS	CA-C-N	6.76	126.74	119.78
1	A	766	HIS	C-N-CA	6.76	126.74	119.78
1	A	1160	ASN	CA-C-N	6.75	128.28	119.84
1	A	1160	ASN	C-N-CA	6.75	128.28	119.84
1	L	22	GLY	CA-C-N	6.75	126.66	119.85
1	L	22	GLY	C-N-CA	6.75	126.66	119.85
1	A	1060	PRO	N-CA-C	6.70	118.87	110.70
1	K	705	GLY	CA-C-N	6.65	126.63	119.78
1	K	705	GLY	C-N-CA	6.65	126.63	119.78
1	D	1220	PRO	N-CA-C	6.64	118.80	110.70
1	L	688	GLN	CA-C-N	6.61	133.60	121.70
1	L	688	GLN	C-N-CA	6.61	133.60	121.70
1	L	546	SER	CA-C-N	6.60	126.54	119.28
1	L	546	SER	C-N-CA	6.60	126.54	119.28
1	L	705	GLY	CA-C-N	6.59	126.57	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	705	GLY	C-N-CA	6.59	126.57	119.78
1	G	1060	PRO	N-CA-C	6.58	118.73	110.70
1	K	406	ASN	CA-C-N	-6.58	111.08	121.87
1	K	406	ASN	C-N-CA	-6.58	111.08	121.87
1	A	939	MET	N-CA-C	6.57	120.39	112.38
1	K	172	LEU	CA-C-N	6.55	126.47	119.85
1	K	172	LEU	C-N-CA	6.55	126.47	119.85
1	D	1113	ARG	N-CA-C	6.54	119.23	111.71
1	L	736	CYS	CA-C-O	-6.53	114.47	121.45
3	I	43	PRO	CA-C-N	6.50	126.42	119.85
3	I	43	PRO	C-N-CA	6.50	126.42	119.85
1	J	546	SER	CA-C-N	6.50	126.43	119.28
1	J	546	SER	C-N-CA	6.50	126.43	119.28
1	J	236	ASN	CA-C-N	-6.48	111.88	120.95
1	J	236	ASN	C-N-CA	-6.48	111.88	120.95
1	L	26	VAL	N-CA-C	6.48	117.26	110.72
1	K	409	TYR	N-CA-C	6.45	118.75	109.14
1	L	195	CYS	CA-C-N	6.44	126.20	119.05
1	L	195	CYS	C-N-CA	6.44	126.20	119.05
1	G	1220	PRO	N-CA-C	6.42	118.53	110.70
1	J	167	HIS	CA-CB-CG	6.39	120.19	113.80
1	G	912	CYS	CA-C-N	6.36	130.35	120.75
1	G	912	CYS	C-N-CA	6.36	130.35	120.75
1	L	188	GLU	CA-C-N	6.36	126.33	119.78
1	L	188	GLU	C-N-CA	6.36	126.33	119.78
1	D	766	HIS	CA-C-N	6.35	126.32	119.78
1	D	766	HIS	C-N-CA	6.35	126.32	119.78
1	G	939	MET	N-CA-C	6.32	120.08	112.38
1	K	484	VAL	CA-C-N	6.29	126.26	119.78
1	K	484	VAL	C-N-CA	6.29	126.26	119.78
1	K	514	VAL	CA-C-N	6.29	126.25	119.78
1	K	514	VAL	C-N-CA	6.29	126.25	119.78
1	L	44	TRP	CA-C-N	6.26	126.18	119.85
1	L	44	TRP	C-N-CA	6.26	126.18	119.85
1	K	604	VAL	N-CA-C	6.21	118.58	109.63
1	K	369	LYS	CB-CA-C	-6.21	106.79	111.20
1	L	484	VAL	N-CA-C	6.21	113.97	108.63
1	L	709	THR	CA-C-N	6.20	126.10	119.28
1	L	709	THR	C-N-CA	6.20	126.10	119.28
1	G	766	HIS	CA-C-N	6.20	126.17	119.78
1	G	766	HIS	C-N-CA	6.20	126.17	119.78
1	G	1160	ASN	CA-C-N	6.20	127.59	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1160	ASN	C-N-CA	6.20	127.59	119.84
1	J	623	VAL	CA-C-N	-6.20	114.52	121.83
1	J	623	VAL	C-N-CA	-6.20	114.52	121.83
1	L	236	ASN	CA-C-N	-6.19	112.57	121.42
1	L	236	ASN	C-N-CA	-6.19	112.57	121.42
1	D	912	CYS	CA-C-N	6.18	130.08	120.75
1	D	912	CYS	C-N-CA	6.18	130.08	120.75
1	D	1193	ALA	CA-C-N	6.18	126.14	119.78
1	D	1193	ALA	C-N-CA	6.18	126.14	119.78
1	G	807	LYS	N-CA-C	-6.17	105.78	113.55
1	L	623	VAL	CA-C-N	-6.15	114.57	121.83
1	L	623	VAL	C-N-CA	-6.15	114.57	121.83
1	K	223	ALA	N-CA-C	6.14	117.64	111.07
1	A	859	SER	CA-C-N	6.13	126.10	119.78
1	A	859	SER	C-N-CA	6.13	126.10	119.78
1	D	924	ILE	CA-C-N	-6.11	110.70	122.06
1	D	924	ILE	C-N-CA	-6.11	110.70	122.06
1	K	399	PHE	N-CA-C	6.06	118.78	110.24
1	L	738	LEU	N-CA-C	6.06	117.52	109.83
1	J	46	ARG	CA-C-N	6.05	126.02	119.78
1	J	46	ARG	C-N-CA	6.05	126.02	119.78
1	K	296	ILE	CA-C-N	6.02	125.93	119.85
1	K	296	ILE	C-N-CA	6.02	125.93	119.85
1	K	600	LEU	N-CA-C	6.02	119.70	111.39
1	D	1060	PRO	N-CA-C	6.00	118.01	110.70
1	J	736	CYS	N-CA-C	-5.97	100.06	108.96
1	J	725	GLU	N-CA-C	5.96	117.77	111.28
1	L	78	GLN	N-CA-C	5.93	117.74	111.28
1	K	321	LEU	N-CA-C	5.92	118.85	110.50
1	L	725	GLU	N-CA-C	5.90	117.72	111.28
1	K	603	CYS	CA-C-N	5.89	128.40	120.50
1	K	603	CYS	C-N-CA	5.89	128.40	120.50
1	L	688	GLN	N-CA-C	5.89	120.57	111.56
1	K	688	GLN	CA-C-N	5.88	132.29	121.70
1	K	688	GLN	C-N-CA	5.88	132.29	121.70
1	G	1058	LEU	N-CA-C	5.88	118.78	109.50
1	J	296	ILE	CA-C-N	5.87	125.78	119.85
1	J	296	ILE	C-N-CA	5.87	125.78	119.85
1	L	271	VAL	N-CA-C	5.87	116.66	111.90
1	K	368	ALA	N-CA-C	5.87	119.75	112.24
1	G	859	SER	CA-C-N	5.80	125.76	119.78
1	G	859	SER	C-N-CA	5.80	125.76	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	92	LYS	N-CA-C	5.80	117.61	111.28
1	G	1044	PHE	CA-CB-CG	-5.80	108.00	113.80
1	K	425	CYS	CA-C-O	5.80	127.59	121.33
1	K	429	SER	CA-C-N	5.79	125.65	119.28
1	K	429	SER	C-N-CA	5.79	125.65	119.28
1	K	585	CYS	CA-C-N	5.78	125.73	119.78
1	K	585	CYS	C-N-CA	5.78	125.73	119.78
1	J	392	THR	CA-C-N	5.77	123.81	119.66
1	J	392	THR	C-N-CA	5.77	123.81	119.66
1	L	649	TYR	CA-C-N	-5.77	113.12	122.81
1	L	649	TYR	C-N-CA	-5.77	113.12	122.81
1	J	657	VAL	CA-C-N	5.75	125.70	119.78
1	J	657	VAL	C-N-CA	5.75	125.70	119.78
1	J	484	VAL	N-CA-C	5.75	113.57	108.63
1	J	271	VAL	N-CA-C	5.74	116.55	111.90
3	F	87	PHE	N-CA-C	5.72	117.73	108.34
1	A	1206	ALA	CA-C-N	5.71	125.66	119.78
1	A	1206	ALA	C-N-CA	5.71	125.66	119.78
1	J	28	SER	CA-C-N	5.71	129.37	120.75
1	J	28	SER	C-N-CA	5.71	129.37	120.75
1	J	323	PHE	N-CA-C	5.69	118.06	109.23
1	G	1219	PRO	N-CA-C	5.69	117.64	110.70
1	D	936	PRO	CA-C-N	5.69	125.59	119.85
1	D	936	PRO	C-N-CA	5.69	125.59	119.85
3	F	92	LYS	N-CA-C	5.68	117.47	111.28
1	J	195	CYS	CA-C-N	5.66	125.33	119.05
1	J	195	CYS	C-N-CA	5.66	125.33	119.05
1	L	323	PHE	N-CA-C	5.66	118.00	109.23
1	L	46	ARG	CA-C-N	5.65	125.60	119.78
1	L	46	ARG	C-N-CA	5.65	125.60	119.78
1	J	649	TYR	CA-C-N	-5.64	113.33	122.81
1	J	649	TYR	C-N-CA	-5.64	113.33	122.81
1	A	871	LEU	N-CA-C	5.62	119.00	111.24
1	G	1217	ASN	N-CA-C	5.62	118.20	107.75
1	K	664	ASP	CA-CB-CG	-5.61	106.99	112.60
1	L	37	GLN	N-CA-C	5.61	118.93	111.75
1	A	916	GLY	CA-C-N	5.60	125.51	119.85
1	A	916	GLY	C-N-CA	5.60	125.51	119.85
1	G	916	GLY	CA-C-N	5.57	125.47	119.85
1	G	916	GLY	C-N-CA	5.57	125.47	119.85
1	K	399	PHE	CB-CA-C	-5.54	100.77	109.70
1	A	1217	ASN	N-CA-C	5.54	117.75	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	392	THR	CA-C-N	5.53	123.64	119.66
1	L	392	THR	C-N-CA	5.53	123.64	119.66
2	E	91	TYR	N-CA-C	5.52	117.39	108.34
1	K	58	TYR	CA-C-N	5.51	125.46	119.78
1	K	58	TYR	C-N-CA	5.51	125.46	119.78
1	G	1156	CYS	CA-C-O	5.51	127.68	121.51
1	G	1157	ASP	CA-CB-CG	5.50	118.10	112.60
1	D	871	LEU	N-CA-C	5.47	118.79	111.24
1	A	924	ILE	CA-C-N	-5.46	112.53	120.29
1	A	924	ILE	C-N-CA	-5.46	112.53	120.29
1	K	590	PHE	N-CA-C	5.46	117.99	111.71
1	K	323	PHE	N-CA-C	5.45	118.33	109.06
1	G	1113	ARG	N-CA-C	5.45	119.77	113.18
1	K	524	SER	CA-C-N	5.44	125.27	119.28
1	K	524	SER	C-N-CA	5.44	125.27	119.28
1	J	58	TYR	CA-C-N	5.44	125.38	119.78
1	J	58	TYR	C-N-CA	5.44	125.38	119.78
1	G	1206	ALA	CA-C-N	5.43	125.37	119.78
1	G	1206	ALA	C-N-CA	5.43	125.37	119.78
1	K	600	LEU	CA-C-N	5.42	131.46	121.70
1	K	600	LEU	C-N-CA	5.42	131.46	121.70
1	G	1156	CYS	O-C-N	-5.41	116.14	122.96
1	K	22	GLY	CA-C-N	5.41	125.35	119.78
1	K	22	GLY	C-N-CA	5.41	125.35	119.78
1	J	373	SER	N-CA-C	5.40	118.12	110.50
1	G	912	CYS	N-CA-C	-5.40	105.50	112.68
3	C	92	LYS	N-CA-C	5.38	117.14	111.28
1	L	184	TYR	CA-C-N	-5.37	113.06	121.87
1	L	184	TYR	C-N-CA	-5.37	113.06	121.87
1	A	1113	ARG	N-CA-C	5.35	119.53	112.89
1	K	709	THR	CA-C-N	5.35	125.16	119.28
1	K	709	THR	C-N-CA	5.35	125.16	119.28
1	D	1044	PHE	CA-CB-CG	-5.34	108.46	113.80
1	J	709	THR	CA-C-N	5.34	125.15	119.28
1	J	709	THR	C-N-CA	5.34	125.15	119.28
1	K	195	CYS	CA-C-N	5.33	124.97	119.05
1	K	195	CYS	C-N-CA	5.33	124.97	119.05
1	K	546	SER	CA-C-N	5.33	125.14	119.28
1	K	546	SER	C-N-CA	5.33	125.14	119.28
1	K	473	PHE	CA-CB-CG	-5.28	108.52	113.80
1	J	503	CYS	CA-C-O	5.28	126.16	119.98
1	K	365	SER	N-CA-C	5.28	117.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	782	ILE	CA-C-N	5.24	125.14	119.85
1	G	782	ILE	C-N-CA	5.24	125.14	119.85
1	G	871	LEU	N-CA-C	5.24	118.47	111.24
1	J	269	ARG	N-CA-C	5.23	116.98	111.28
1	K	469	TYR	N-CA-C	5.20	117.64	108.75
1	J	383	CYS	CB-CA-C	-5.20	102.46	110.26
1	D	870	ASN	N-CA-C	5.20	117.03	111.36
1	A	1044	PHE	CA-CB-CG	-5.19	108.61	113.80
1	D	807	LYS	N-CA-C	-5.18	107.02	113.55
1	A	807	LYS	N-CA-C	-5.18	105.79	112.68
1	K	606	TYR	N-CA-C	5.18	116.94	109.07
1	J	223	ALA	N-CA-C	5.18	116.61	111.07
1	L	396	VAL	N-CA-C	5.18	118.32	111.17
1	D	1206	ALA	CA-C-N	5.16	125.10	119.78
1	D	1206	ALA	C-N-CA	5.16	125.10	119.78
1	A	782	ILE	CA-C-N	5.16	125.06	119.85
1	A	782	ILE	C-N-CA	5.16	125.06	119.85
1	G	1124	VAL	N-CA-C	5.16	116.89	109.51
1	L	615	GLY	N-CA-C	5.16	118.11	110.42
1	K	341	PHE	N-CA-C	5.15	116.97	111.36
1	L	185	CYS	N-CA-C	5.14	116.62	108.96
1	D	970	ILE	CA-C-N	5.11	125.05	119.78
1	D	970	ILE	C-N-CA	5.11	125.05	119.78
1	J	26	VAL	N-CA-C	5.11	115.88	110.72
1	J	396	VAL	N-CA-C	5.11	118.22	111.17
1	L	172	LEU	CA-C-N	5.10	125.00	119.85
1	L	172	LEU	C-N-CA	5.10	125.00	119.85
1	J	615	GLY	N-CA-C	5.09	118.00	110.42
1	K	46	ARG	CA-C-N	5.08	125.02	119.78
1	K	46	ARG	C-N-CA	5.08	125.02	119.78
1	D	776	SER	N-CA-C	5.08	119.35	113.20
1	A	1219	PRO	N-CA-C	5.08	116.89	110.70
3	I	87	PHE	N-CA-C	5.08	117.34	108.76
1	L	736	CYS	CA-CB-SG	5.07	126.06	114.40
1	L	58	TYR	CA-C-N	5.06	124.99	119.78
1	L	58	TYR	C-N-CA	5.06	124.99	119.78
1	J	44	TRP	CA-C-N	5.06	124.96	119.85
1	J	44	TRP	C-N-CA	5.06	124.96	119.85
1	L	296	ILE	CA-C-N	5.05	124.95	119.85
1	L	296	ILE	C-N-CA	5.05	124.95	119.85
1	D	1124	VAL	N-CA-C	5.05	116.73	109.51
1	J	101	PHE	CB-CA-C	-5.04	102.76	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	677	VAL	N-CA-C	5.03	117.34	111.05
1	K	302	SER	CA-C-N	5.03	127.24	120.50
1	K	302	SER	C-N-CA	5.03	127.24	120.50
1	J	524	SER	CA-C-N	5.03	124.63	119.05
1	J	524	SER	C-N-CA	5.03	124.63	119.05
1	J	672	THR	N-CA-C	5.03	116.84	109.24
1	L	320	PRO	CA-C-N	5.03	130.12	120.97
1	L	320	PRO	C-N-CA	5.03	130.12	120.97
1	L	672	THR	N-CA-C	5.02	117.31	109.52
3	C	87	PHE	N-CA-C	5.02	117.24	108.76
1	L	373	SER	N-CA-C	5.02	117.58	110.50
1	L	606	TYR	N-CA-C	5.02	116.81	109.24
1	K	533	THR	CA-C-N	-5.01	116.11	122.37
1	K	533	THR	C-N-CA	-5.01	116.11	122.37
1	D	798	THR	N-CA-C	5.01	116.80	109.24
1	J	384	ASP	N-CA-C	5.00	117.42	108.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3531	0	3454	17	0
1	D	3538	0	3463	21	0
1	G	3527	0	3453	15	0
1	J	5645	0	5413	82	0
1	K	5645	0	5413	61	0
1	L	5638	0	5408	98	0
2	B	948	0	904	0	0
2	E	948	0	904	0	0
2	H	948	0	904	1	0
3	C	835	0	816	3	0
3	F	835	0	816	1	0
3	I	835	0	816	2	0
All	All	32873	0	31764	300	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:371:SER:CB	1:L:604:VAL:HG12	1.25	1.63
1:J:371:SER:CB	1:J:604:VAL:HG12	1.17	1.59
1:L:506:PHE:CE2	1:L:555:VAL:CG2	1.77	1.54
1:L:506:PHE:CE2	1:L:555:VAL:HG21	0.85	1.37
1:L:506:PHE:HE2	1:L:555:VAL:CG2	1.20	1.36
1:J:371:SER:HB3	1:J:604:VAL:CG1	1.52	1.34
1:J:371:SER:CB	1:J:604:VAL:CG1	2.01	1.33
1:D:905:TYR:OH	1:D:936:PRO:CA	1.78	1.31
1:L:371:SER:HB3	1:L:604:VAL:CG1	1.60	1.31
1:L:384:ASP:O	1:L:404:PHE:CZ	1.83	1.31
1:L:506:PHE:CD2	1:L:555:VAL:HG21	1.69	1.27
1:L:371:SER:CB	1:L:604:VAL:CG1	2.10	1.26
1:L:506:PHE:CD2	1:L:555:VAL:CG2	2.22	1.21
1:D:905:TYR:OH	1:D:936:PRO:HA	1.47	1.13
1:J:371:SER:OG	1:J:604:VAL:CG1	1.96	1.13
1:K:477:THR:OG1	1:K:573:ILE:O	1.65	1.10
1:J:185:CYS:HB2	1:J:237:CYS:HA	1.34	1.09
1:L:371:SER:OG	1:L:604:VAL:CG1	1.99	1.09
1:K:506:PHE:CE1	1:K:513:GLU:OE2	2.06	1.08
1:D:905:TYR:OH	1:D:936:PRO:N	1.87	1.07
1:J:371:SER:OG	1:J:604:VAL:HG12	1.52	1.02
1:L:371:SER:OG	1:L:604:VAL:HG12	1.55	1.02
1:J:371:SER:CA	1:J:604:VAL:HG12	1.89	1.01
1:A:868:ASP:OD2	1:A:995:LYS:NZ	1.94	0.99
1:J:185:CYS:SG	1:J:186:ILE:N	2.29	0.99
1:J:187:LEU:HD21	1:J:228:PHE:HZ	1.25	0.99
1:L:371:SER:HB3	1:L:604:VAL:HG12	0.99	0.97
1:L:384:ASP:CB	1:L:404:PHE:HE2	1.75	0.97
1:L:384:ASP:O	1:L:404:PHE:CE2	2.18	0.97
1:L:621:THR:O	1:L:648:TYR:HD2	1.45	0.96
1:J:185:CYS:SG	1:J:235:ARG:O	2.23	0.96
1:L:372:GLY:O	1:L:604:VAL:HB	1.66	0.95
1:J:371:SER:HB3	1:J:604:VAL:HG12	0.98	0.95
1:D:905:TYR:CZ	1:D:936:PRO:HB3	2.03	0.92
1:L:506:PHE:CD2	1:L:555:VAL:HG23	2.03	0.92
1:J:185:CYS:CB	1:J:237:CYS:HA	2.00	0.90
1:L:371:SER:CA	1:L:604:VAL:HG12	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:CYS:HB2	1:J:237:CYS:CA	2.02	0.89
1:J:372:GLY:O	1:J:604:VAL:HB	1.74	0.87
1:J:185:CYS:HG	1:J:237:CYS:HG	1.08	0.87
1:J:184:TYR:CE1	1:J:286:VAL:HG11	2.11	0.86
1:L:425:CYS:SG	1:L:478:CYS:CB	2.66	0.84
1:K:477:THR:HB	1:K:574:THR:HB	1.60	0.83
1:L:506:PHE:HE2	1:L:555:VAL:HG22	1.40	0.83
1:L:621:THR:O	1:L:648:TYR:CD2	2.30	0.83
1:J:371:SER:HB3	1:J:604:VAL:HG13	1.57	0.83
1:K:471:GLN:HG2	1:K:477:THR:HG21	1.61	0.82
1:L:425:CYS:CB	1:L:478:CYS:SG	2.68	0.81
1:L:425:CYS:SG	1:L:478:CYS:HB3	2.19	0.81
1:L:425:CYS:HB3	1:L:478:CYS:SG	2.21	0.81
1:L:384:ASP:O	1:L:404:PHE:HZ	1.58	0.80
1:K:471:GLN:CG	1:K:477:THR:HG21	2.13	0.79
1:J:371:SER:C	1:J:604:VAL:HG12	2.08	0.79
1:K:477:THR:HB	1:K:574:THR:CB	2.11	0.79
1:J:184:TYR:OH	1:J:288:ASP:OD2	2.01	0.79
1:J:184:TYR:CG	1:J:286:VAL:HG21	2.18	0.78
1:L:372:GLY:O	1:L:604:VAL:CB	2.31	0.78
1:D:905:TYR:HH	1:D:936:PRO:HA	1.49	0.77
1:G:912:CYS:HG	1:G:925:CYS:HG	1.30	0.77
1:L:477:THR:HB	1:L:574:THR:HG22	1.65	0.77
1:K:506:PHE:CZ	1:K:513:GLU:OE2	2.37	0.76
1:L:602:ASN:O	1:L:616:VAL:HB	1.84	0.76
1:J:187:LEU:HD21	1:J:228:PHE:CZ	2.17	0.75
1:L:384:ASP:CB	1:L:404:PHE:CE2	2.65	0.75
1:L:425:CYS:CB	1:L:478:CYS:HG	2.00	0.74
1:K:477:THR:CB	1:K:573:ILE:O	2.35	0.74
1:K:369:LYS:O	1:K:369:LYS:HG2	1.88	0.74
1:D:905:TYR:OH	1:D:936:PRO:CB	2.36	0.72
1:J:372:GLY:O	1:J:604:VAL:CB	2.37	0.72
1:K:477:THR:HG1	1:K:573:ILE:C	1.92	0.72
1:L:381:VAL:HG11	1:L:407:CYS:HA	1.70	0.72
1:L:621:THR:HG22	1:L:622:ALA:N	2.03	0.72
1:D:905:TYR:CZ	1:D:936:PRO:CB	2.73	0.72
1:J:602:ASN:O	1:J:616:VAL:HB	1.90	0.71
1:K:471:GLN:CD	1:K:477:THR:HG21	2.17	0.70
1:L:384:ASP:HB2	1:L:404:PHE:HE2	1.54	0.70
1:L:371:SER:HB3	1:L:604:VAL:HG13	1.71	0.70
1:L:477:THR:CG2	1:L:574:THR:HG22	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:CYS:CB	1:J:237:CYS:SG	2.81	0.69
1:L:371:SER:C	1:L:604:VAL:HG12	2.17	0.69
1:J:185:CYS:CB	1:J:237:CYS:HG	2.05	0.69
1:L:506:PHE:HD2	1:L:555:VAL:HG23	1.56	0.68
1:L:406:ASN:HA	1:L:583:SER:HB2	1.76	0.67
1:J:185:CYS:HB2	1:J:237:CYS:CB	2.26	0.66
1:K:506:PHE:CD1	1:K:513:GLU:OE2	2.48	0.66
1:J:371:SER:OG	1:J:604:VAL:HG11	1.92	0.66
1:L:477:THR:CB	1:L:574:THR:HG22	2.26	0.65
1:K:477:THR:HG1	1:K:478:CYS:H	1.45	0.65
1:J:184:TYR:CD1	1:J:286:VAL:HG21	2.31	0.64
1:K:621:THR:O	1:K:648:TYR:HD2	1.80	0.64
1:K:621:THR:HG22	1:K:622:ALA:N	2.11	0.64
1:L:425:CYS:HG	1:L:478:CYS:CB	2.06	0.64
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.80	0.64
1:J:184:TYR:HB3	1:J:239:PHE:HB2	1.80	0.63
1:K:383:CYS:SG	1:K:409:TYR:HB3	2.38	0.63
1:J:186:ILE:HG22	1:J:187:LEU:N	2.13	0.63
1:L:384:ASP:CA	1:L:404:PHE:HE2	2.12	0.62
1:L:382:GLU:HA	1:L:382:GLU:OE1	1.99	0.62
1:J:371:SER:C	1:J:604:VAL:CG1	2.73	0.62
1:A:897:LYS:HE2	1:A:897:LYS:HA	1.81	0.62
1:J:184:TYR:HD2	1:J:239:PHE:HD1	1.45	0.62
1:J:185:CYS:SG	1:J:237:CYS:HA	2.39	0.61
1:L:384:ASP:HB3	1:L:404:PHE:HE2	1.65	0.61
1:J:184:TYR:CZ	1:J:286:VAL:CG1	2.83	0.61
1:L:384:ASP:HB3	1:L:404:PHE:CE2	2.34	0.61
1:L:599:GLN:C	1:L:600:LEU:HG	2.24	0.61
1:L:477:THR:HG22	1:L:574:THR:HB	1.83	0.61
1:K:738:LEU:HD12	1:K:739:PRO:HD3	1.82	0.60
1:J:184:TYR:CZ	1:J:286:VAL:HG13	2.37	0.60
1:L:621:THR:CG2	1:L:622:ALA:N	2.64	0.59
1:L:371:SER:OG	1:L:604:VAL:HG11	1.97	0.59
1:J:599:GLN:C	1:J:600:LEU:HG	2.25	0.59
1:J:616:VAL:HG13	1:J:616:VAL:O	2.03	0.59
1:J:184:TYR:CD2	1:J:239:PHE:HD1	2.21	0.58
1:L:602:ASN:O	1:L:616:VAL:CB	2.52	0.58
1:J:184:TYR:CD2	1:J:286:VAL:CG2	2.88	0.57
1:L:616:VAL:O	1:L:616:VAL:HG13	2.03	0.57
1:J:184:TYR:CE2	1:J:286:VAL:HG22	2.41	0.56
1:J:187:LEU:CD2	1:J:228:PHE:HZ	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:506:PHE:CE2	1:L:555:VAL:HG22	2.20	0.56
1:J:372:GLY:O	1:J:604:VAL:CG2	2.54	0.56
1:J:602:ASN:O	1:J:616:VAL:CB	2.54	0.56
1:K:478:CYS:O	1:K:479:LEU:HG	2.06	0.55
1:L:240:MET:SD	1:L:240:MET:C	2.89	0.55
1:D:1175:THR:HG23	1:D:1175:THR:O	2.07	0.55
1:D:905:TYR:CZ	1:D:936:PRO:HA	2.40	0.55
1:K:621:THR:CG2	1:K:622:ALA:N	2.70	0.54
1:L:384:ASP:CA	1:L:404:PHE:CE2	2.91	0.54
1:J:184:TYR:CE1	1:J:286:VAL:CG1	2.86	0.53
1:G:1175:THR:HG23	1:G:1175:THR:O	2.07	0.53
1:A:1175:THR:HG23	1:A:1175:THR:O	2.09	0.53
1:L:384:ASP:C	1:L:404:PHE:CE2	2.85	0.53
1:J:184:TYR:HD2	1:J:239:PHE:CD1	2.24	0.53
1:L:384:ASP:HB2	1:L:404:PHE:CE2	2.40	0.53
1:L:67:ILE:HG13	1:L:67:ILE:O	2.08	0.53
1:K:172:LEU:O	1:K:172:LEU:HG	2.08	0.53
1:G:875:GLU:OE1	1:G:875:GLU:N	2.35	0.53
1:J:186:ILE:C	1:J:187:LEU:HD12	2.34	0.53
1:A:875:GLU:OE1	1:A:875:GLU:N	2.36	0.53
1:K:477:THR:HA	1:K:574:THR:HA	1.91	0.53
1:L:381:VAL:CG1	1:L:407:CYS:HA	2.39	0.52
1:L:621:THR:CG2	1:L:622:ALA:H	2.22	0.52
1:J:185:CYS:SG	1:J:237:CYS:CA	2.98	0.52
1:L:342:ASN:C	1:L:342:ASN:OD1	2.53	0.51
1:J:184:TYR:CD2	1:J:286:VAL:HG22	2.45	0.51
1:K:738:LEU:HD12	1:K:739:PRO:CD	2.41	0.51
1:A:875:GLU:O	1:A:875:GLU:HG2	2.09	0.51
1:L:399:PHE:O	1:L:399:PHE:CD1	2.64	0.51
1:G:826:GLN:OE1	1:G:826:GLN:N	2.27	0.50
1:K:477:THR:HG1	1:K:478:CYS:N	2.09	0.50
1:K:606:TYR:CD1	1:K:606:TYR:C	2.88	0.50
1:J:665:LYS:HD3	1:J:665:LYS:C	2.37	0.49
1:L:256:ILE:HG23	1:L:256:ILE:O	2.11	0.49
1:J:184:TYR:CD2	1:J:286:VAL:HG21	2.47	0.49
1:L:477:THR:CG2	1:L:574:THR:CG2	2.90	0.49
3:C:1:ASP:C	3:C:1:ASP:OD1	2.56	0.49
1:D:905:TYR:OH	1:D:935:LEU:C	2.54	0.49
1:G:912:CYS:SG	1:K:655:VAL:HG12	2.52	0.49
1:K:477:THR:OG1	1:K:478:CYS:N	2.44	0.49
1:L:372:GLY:O	1:L:604:VAL:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1001:PHE:C	1:G:1001:PHE:CD2	2.91	0.49
1:J:166:ASN:O	1:J:186:ILE:HG23	2.11	0.49
1:L:371:SER:HG	1:L:604:VAL:CG1	2.23	0.49
1:A:1124:VAL:HG13	1:A:1124:VAL:O	2.13	0.48
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.56	0.48
1:G:897:LYS:HE2	1:G:897:LYS:HA	1.95	0.48
1:J:186:ILE:CG2	1:J:187:LEU:N	2.75	0.48
1:K:471:GLN:HG2	1:K:477:THR:CG2	2.38	0.48
1:L:477:THR:HG22	1:L:574:THR:CB	2.42	0.48
1:K:477:THR:CA	1:K:573:ILE:O	2.61	0.48
1:L:78:GLN:CD	1:L:78:GLN:C	2.81	0.48
1:G:875:GLU:O	1:G:875:GLU:HG2	2.13	0.48
1:L:371:SER:CB	1:L:604:VAL:HG13	2.29	0.48
1:L:437:CYS:SG	1:L:584:VAL:O	2.72	0.48
1:L:395:GLN:HA	1:L:395:GLN:OE1	2.14	0.47
1:A:1120:GLY:O	1:A:1121:THR:OG1	2.31	0.47
1:L:479:LEU:C	1:L:480:ILE:HG13	2.40	0.47
1:J:694:ARG:HA	1:J:694:ARG:NE	2.29	0.47
1:J:605:GLU:HA	1:J:614:ARG:HA	1.96	0.47
1:K:596:ILE:HD12	1:K:596:ILE:C	2.39	0.47
1:L:382:GLU:O	1:L:407:CYS:HB2	2.15	0.47
1:L:605:GLU:HA	1:L:614:ARG:HA	1.96	0.47
1:L:694:ARG:NE	1:L:694:ARG:HA	2.29	0.47
1:L:694:ARG:HA	1:L:694:ARG:HE	1.80	0.47
1:A:1001:PHE:C	1:A:1001:PHE:CD2	2.93	0.47
1:J:372:GLY:O	1:J:604:VAL:HG21	2.14	0.47
1:J:142:LYS:NZ	1:J:142:LYS:HB3	2.29	0.47
1:L:438:TYR:O	1:L:584:VAL:HB	2.14	0.47
1:J:49:ASP:C	1:J:49:ASP:OD1	2.58	0.46
1:K:478:CYS:N	1:K:573:ILE:O	2.40	0.46
1:L:371:SER:C	1:L:604:VAL:CG1	2.87	0.46
3:C:92:LYS:HD3	3:C:92:LYS:C	2.41	0.46
1:J:371:SER:C	1:J:604:VAL:HB	2.40	0.46
1:K:439:SER:HA	1:K:582:ASN:HA	1.98	0.46
1:K:326:ASP:C	1:K:326:ASP:OD1	2.56	0.46
1:K:409:TYR:CD1	1:K:409:TYR:C	2.94	0.46
1:J:130:VAL:O	1:J:130:VAL:HG12	2.16	0.46
1:J:185:CYS:CB	1:J:237:CYS:CA	2.79	0.46
1:K:395:GLN:OE1	1:K:395:GLN:HA	2.14	0.46
1:K:731:LEU:HB2	1:K:735:LEU:HB3	1.97	0.46
1:A:806:CYS:SG	1:A:806:CYS:O	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:ASN:O	1:J:186:ILE:HG12	2.15	0.46
1:J:689:TYR:CD1	1:J:689:TYR:C	2.94	0.46
1:D:809:TYR:CD2	1:D:809:TYR:C	2.94	0.46
1:L:665:LYS:HD3	1:L:665:LYS:C	2.40	0.46
1:L:719:ASN:OD1	1:L:719:ASN:C	2.59	0.46
1:G:777:TYR:N	1:G:777:TYR:CD2	2.84	0.45
1:L:477:THR:C	1:L:478:CYS:SG	3.00	0.45
1:D:875:GLU:HB3	1:D:886:ALA:HB3	1.97	0.45
3:I:92:LYS:HD3	3:I:92:LYS:C	2.41	0.45
1:K:477:THR:HB	1:K:574:THR:CA	2.45	0.45
1:J:371:SER:CB	1:J:604:VAL:HG13	2.21	0.45
1:K:523:TYR:N	1:K:523:TYR:CD1	2.84	0.45
1:L:372:GLY:C	1:L:604:VAL:HB	2.39	0.45
1:J:372:GLY:C	1:J:604:VAL:HB	2.39	0.45
1:L:664:ASP:OD1	1:L:664:ASP:C	2.57	0.45
1:K:621:THR:O	1:K:648:TYR:CD2	2.65	0.45
1:L:615:GLY:HA2	1:L:654:CYS:SG	2.57	0.45
1:D:806:CYS:O	1:D:806:CYS:SG	2.74	0.45
1:J:184:TYR:CD2	1:J:239:PHE:CD1	3.03	0.45
1:K:130:VAL:O	1:K:130:VAL:HG12	2.17	0.45
1:D:905:TYR:CE2	1:D:936:PRO:HB3	2.51	0.44
1:D:1036:LEU:HA	1:D:1036:LEU:HD23	1.74	0.44
1:G:1160:ASN:OD1	1:G:1160:ASN:C	2.61	0.44
1:K:378:ALA:HB1	1:K:379:GLU:HA	1.99	0.44
1:L:240:MET:SD	1:L:240:MET:O	2.75	0.44
1:K:633:ASP:OD1	1:K:633:ASP:C	2.58	0.44
1:J:371:SER:C	1:J:604:VAL:CB	2.90	0.44
3:I:1:ASP:OD1	3:I:1:ASP:C	2.56	0.44
1:K:49:ASP:OD1	1:K:49:ASP:C	2.59	0.44
1:J:615:GLY:HA2	1:J:654:CYS:SG	2.58	0.44
1:L:621:THR:HG22	1:L:622:ALA:H	1.76	0.44
1:L:440:SER:HA	1:L:584:VAL:HG21	2.00	0.44
1:A:1062:GLU:N	1:A:1062:GLU:OE1	2.51	0.44
3:F:2:ILE:N	3:F:2:ILE:HD12	2.32	0.44
1:L:49:ASP:OD1	1:L:49:ASP:C	2.61	0.44
1:A:774:ASN:OD1	1:A:774:ASN:C	2.61	0.44
1:K:172:LEU:N	1:K:172:LEU:HD23	2.33	0.44
1:J:440:SER:HA	1:J:584:VAL:HG21	2.00	0.43
1:K:174:ASP:OD1	1:K:174:ASP:C	2.60	0.43
1:K:410:ASN:C	1:K:410:ASN:OD1	2.61	0.43
1:K:590:PHE:O	1:K:590:PHE:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1001:PHE:C	1:D:1001:PHE:CD2	2.97	0.43
1:J:438:TYR:O	1:J:584:VAL:HB	2.18	0.43
1:K:689:TYR:C	1:K:689:TYR:CD1	2.96	0.43
1:J:228:PHE:CD2	1:J:228:PHE:C	2.96	0.43
1:G:932:TYR:HD1	1:G:932:TYR:HA	1.45	0.43
1:K:477:THR:OG1	1:K:573:ILE:C	2.53	0.43
1:A:826:GLN:OE1	1:A:826:GLN:N	2.31	0.43
1:L:384:ASP:C	1:L:404:PHE:CZ	2.84	0.43
1:A:965:SER:OG	1:A:966:SER:N	2.52	0.42
1:G:806:CYS:O	1:G:806:CYS:SG	2.77	0.42
1:A:826:GLN:H	1:A:826:GLN:CD	2.23	0.42
1:L:330:ASP:OD1	1:L:330:ASP:C	2.62	0.42
1:G:1060:PRO:HA	1:G:1063:GLN:HB3	2.00	0.42
1:K:732:GLY:O	1:K:735:LEU:HB2	2.19	0.42
1:J:633:ASP:C	1:J:633:ASP:OD1	2.62	0.42
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	2.00	0.42
1:K:399:PHE:O	1:K:523:TYR:OH	2.36	0.42
1:L:633:ASP:OD1	1:L:633:ASP:C	2.62	0.42
1:G:1124:VAL:O	1:G:1124:VAL:HG13	2.19	0.42
2:H:61:GLN:C	2:H:61:GLN:CD	2.87	0.42
1:J:330:ASP:OD1	1:J:330:ASP:C	2.63	0.42
3:C:28:TYR:N	3:C:28:TYR:CD1	2.86	0.42
1:G:965:SER:OG	1:G:966:SER:N	2.52	0.42
1:J:371:SER:HG	1:J:604:VAL:CG1	2.21	0.42
1:A:872:THR:O	1:A:872:THR:HG22	2.19	0.42
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.20	0.42
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.20	0.42
1:J:371:SER:O	1:J:604:VAL:HB	2.19	0.42
1:L:616:VAL:O	1:L:616:VAL:CG1	2.68	0.42
1:L:185:CYS:SG	1:L:186:ILE:N	2.93	0.41
1:L:506:PHE:CE2	1:L:555:VAL:CB	2.88	0.41
1:K:172:LEU:HD23	1:K:172:LEU:H	1.85	0.41
1:K:645:ASP:OD1	1:K:645:ASP:C	2.63	0.41
1:D:777:TYR:N	1:D:777:TYR:CD2	2.88	0.41
1:J:67:ILE:O	1:J:67:ILE:HG23	2.19	0.41
1:J:384:ASP:OD1	1:J:384:ASP:C	2.64	0.41
1:J:184:TYR:CE2	1:J:286:VAL:CG2	3.04	0.41
1:J:603:CYS:O	1:J:603:CYS:SG	2.79	0.41
1:K:130:VAL:O	1:K:130:VAL:CG1	2.69	0.41
1:K:209:THR:O	1:K:209:THR:HG22	2.20	0.41
1:K:621:THR:CG2	1:K:622:ALA:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:VAL:O	1:L:130:VAL:HG12	2.20	0.41
1:L:477:THR:O	1:L:478:CYS:SG	2.79	0.41
1:K:269:ARG:HD3	1:K:269:ARG:C	2.46	0.41
1:K:677:VAL:O	1:K:677:VAL:HG22	2.20	0.41
1:D:1124:VAL:O	1:D:1124:VAL:HG13	2.21	0.41
1:J:719:ASN:OD1	1:J:719:ASN:C	2.63	0.41
1:K:739:PRO:O	1:K:740:ASP:C	2.63	0.40
1:D:775:SER:OG	1:D:776:SER:N	2.53	0.40
1:L:603:CYS:SG	1:L:603:CYS:O	2.79	0.40
1:L:645:ASP:OD1	1:L:645:ASP:C	2.64	0.40
1:K:427:GLN:HB2	1:K:476:PRO:HB3	2.04	0.40
1:L:604:VAL:O	1:L:604:VAL:HG23	2.21	0.40
1:L:606:TYR:CD1	1:L:606:TYR:C	3.00	0.40
1:J:130:VAL:O	1:J:130:VAL:CG1	2.68	0.40
1:J:443:LEU:HD23	1:J:443:LEU:C	2.46	0.40
1:K:478:CYS:HB3	1:K:479:LEU:H	1.73	0.40
1:K:670:HIS:N	1:K:670:HIS:CD2	2.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	457/1329 (34%)	439 (96%)	15 (3%)	3 (1%)	18	55
1	D	458/1329 (34%)	441 (96%)	12 (3%)	5 (1%)	11	45
1	G	456/1329 (34%)	438 (96%)	15 (3%)	3 (1%)	18	55
1	J	722/1329 (54%)	685 (95%)	34 (5%)	3 (0%)	30	67
1	K	722/1329 (54%)	688 (95%)	30 (4%)	4 (1%)	21	58
1	L	721/1329 (54%)	685 (95%)	32 (4%)	4 (1%)	21	58
2	B	117/233 (50%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
2	H	117/233 (50%)	115 (98%)	2 (2%)	0	100	100
3	C	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	14	49
3	F	109/218 (50%)	105 (96%)	2 (2%)	2 (2%)	6	33
3	I	109/218 (50%)	104 (95%)	4 (4%)	1 (1%)	14	49
All	All	4214/9327 (45%)	4034 (96%)	154 (4%)	26 (1%)	23	58

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	940	ASP
1	A	961	THR
1	D	961	THR
1	D	965	SER
1	G	940	ASP
1	J	718	VAL
1	K	718	VAL
1	L	718	VAL
3	C	77	PRO
1	D	905	TYR
1	G	961	THR
3	I	77	PRO
1	A	1220	PRO
1	D	1220	PRO
3	F	31	SER
3	F	77	PRO
1	G	1220	PRO
1	K	378	ALA
1	D	956	ALA
1	J	368	ALA
1	K	629	ARG
1	L	368	ALA
1	K	44	TRP
1	L	385	PHE
1	J	586	PRO
1	L	586	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	384/1148 (33%)	383 (100%)	1 (0%)	86	84
1	K	633/1148 (55%)	632 (100%)	1 (0%)	87	85
1	L	632/1148 (55%)	629 (100%)	3 (0%)	81	81
All	All	1649/3444 (48%)	1644 (100%)	5 (0%)	84	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	600	LEU
1	K	477	THR
1	L	383	CYS
1	L	384	ASP
1	L	600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	319	GLN
1	J	346	GLN
1	J	475	ASN
1	K	36	GLN
1	K	37	GLN
1	K	78	GLN
1	K	199	ASN
1	K	521	ASN
1	K	618	GLN
1	K	628	GLN
1	L	78	GLN
1	L	111	GLN
1	L	346	GLN
1	L	566	GLN
1	L	618	GLN
1	L	636	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

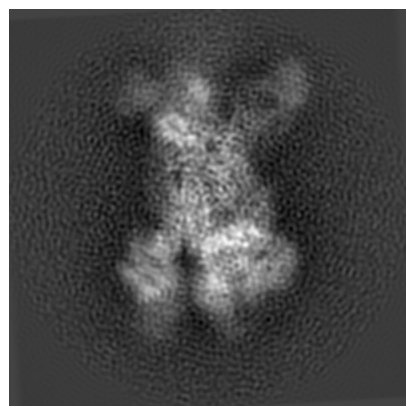
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8786. These allow visual inspection of the internal detail of the map and identification of artifacts.

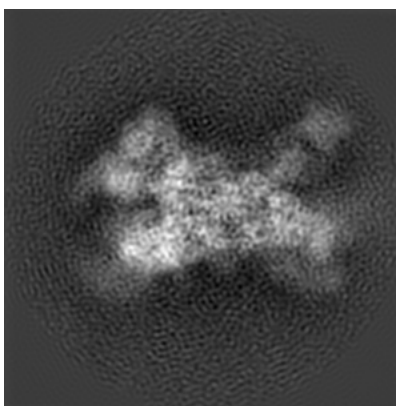
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

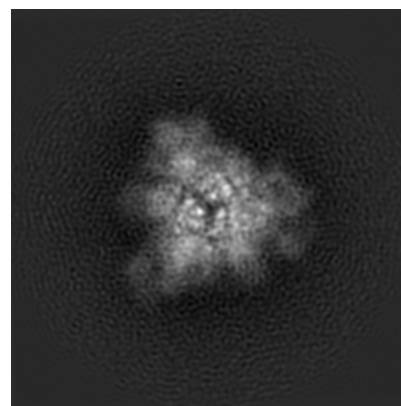
6.1.1 Primary map



X

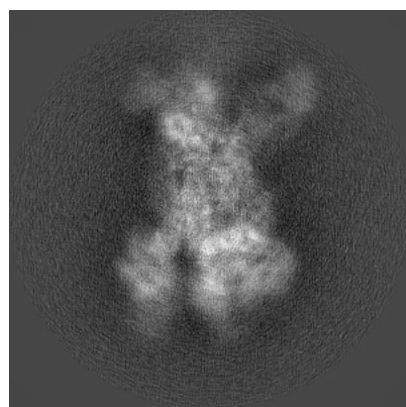


Y

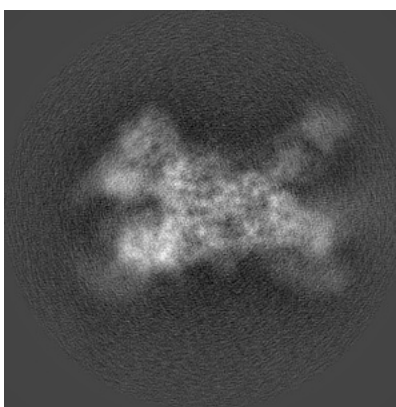


Z

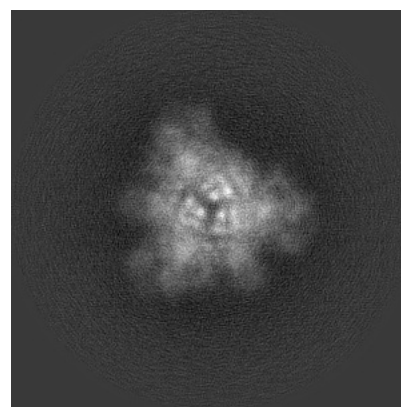
6.1.2 Raw map



X



Y

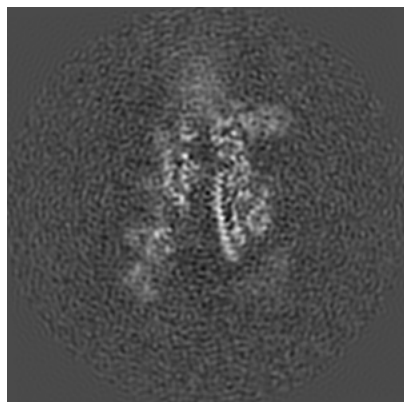


Z

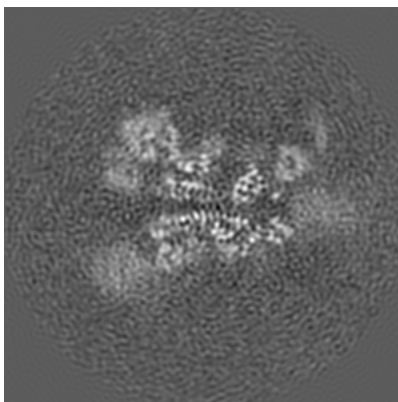
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

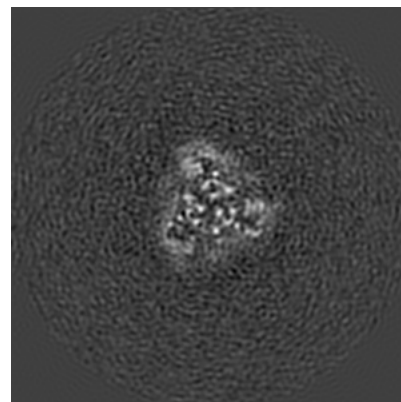
6.2.1 Primary map



X Index: 152

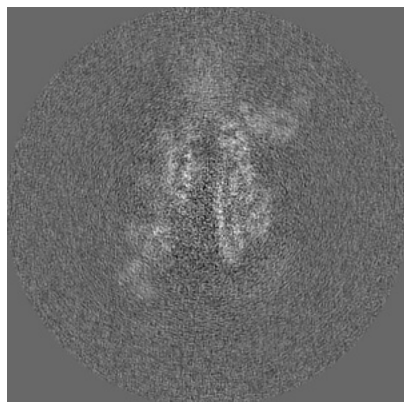


Y Index: 152

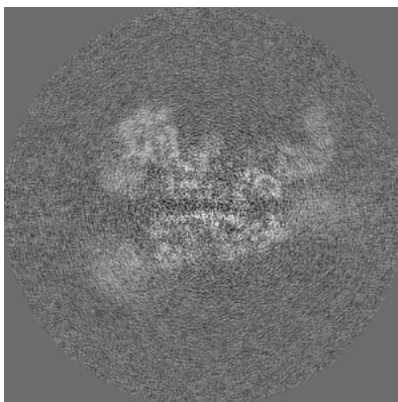


Z Index: 152

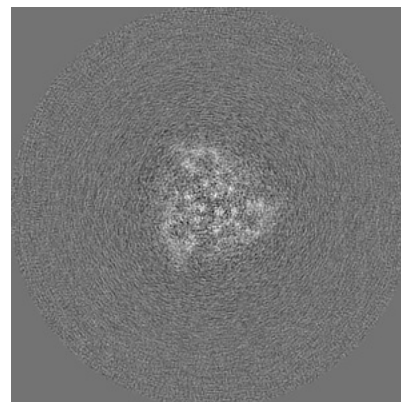
6.2.2 Raw map



X Index: 152



Y Index: 152

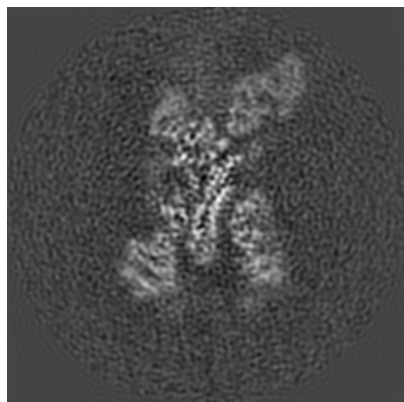


Z Index: 152

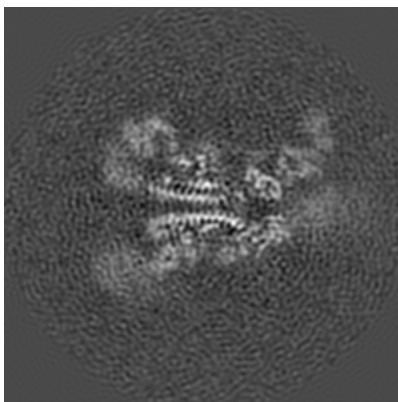
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

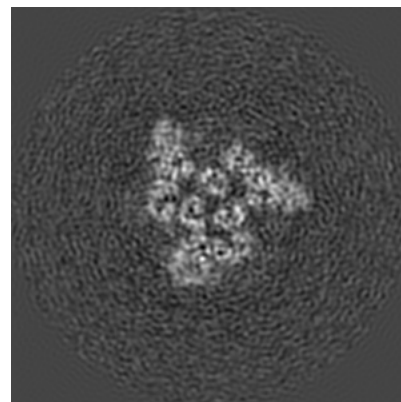
6.3.1 Primary map



X Index: 134

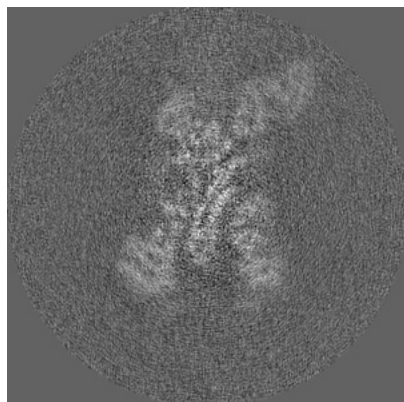


Y Index: 149

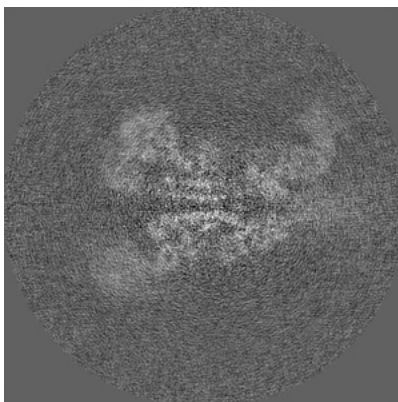


Z Index: 124

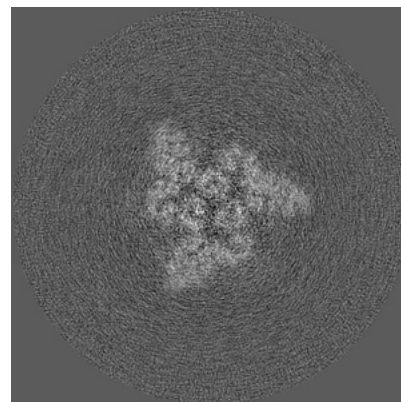
6.3.2 Raw map



X Index: 135



Y Index: 150

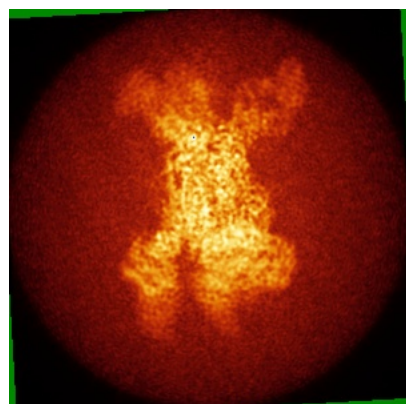


Z Index: 124

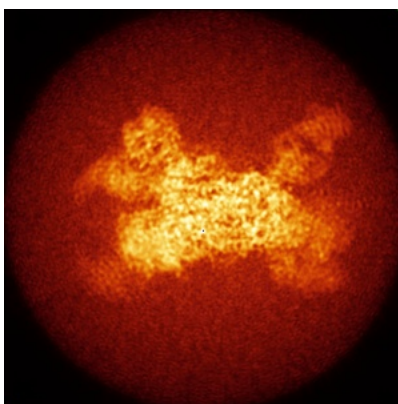
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

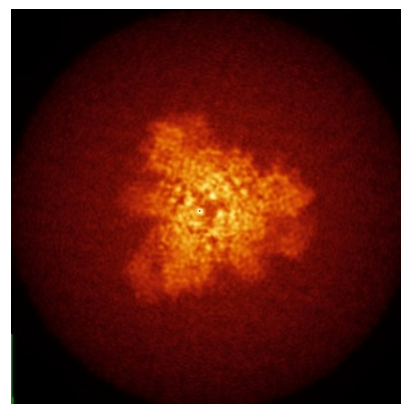
6.4.1 Primary map



X

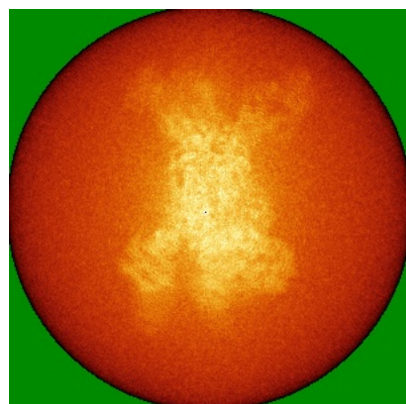


Y

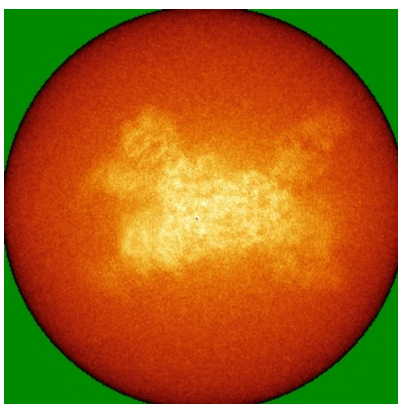


Z

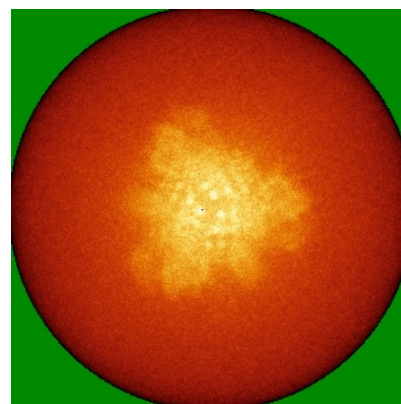
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



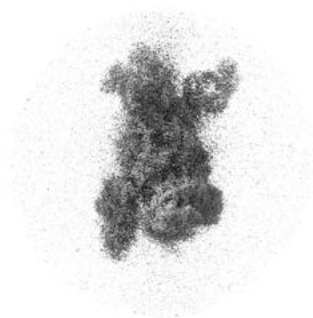
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

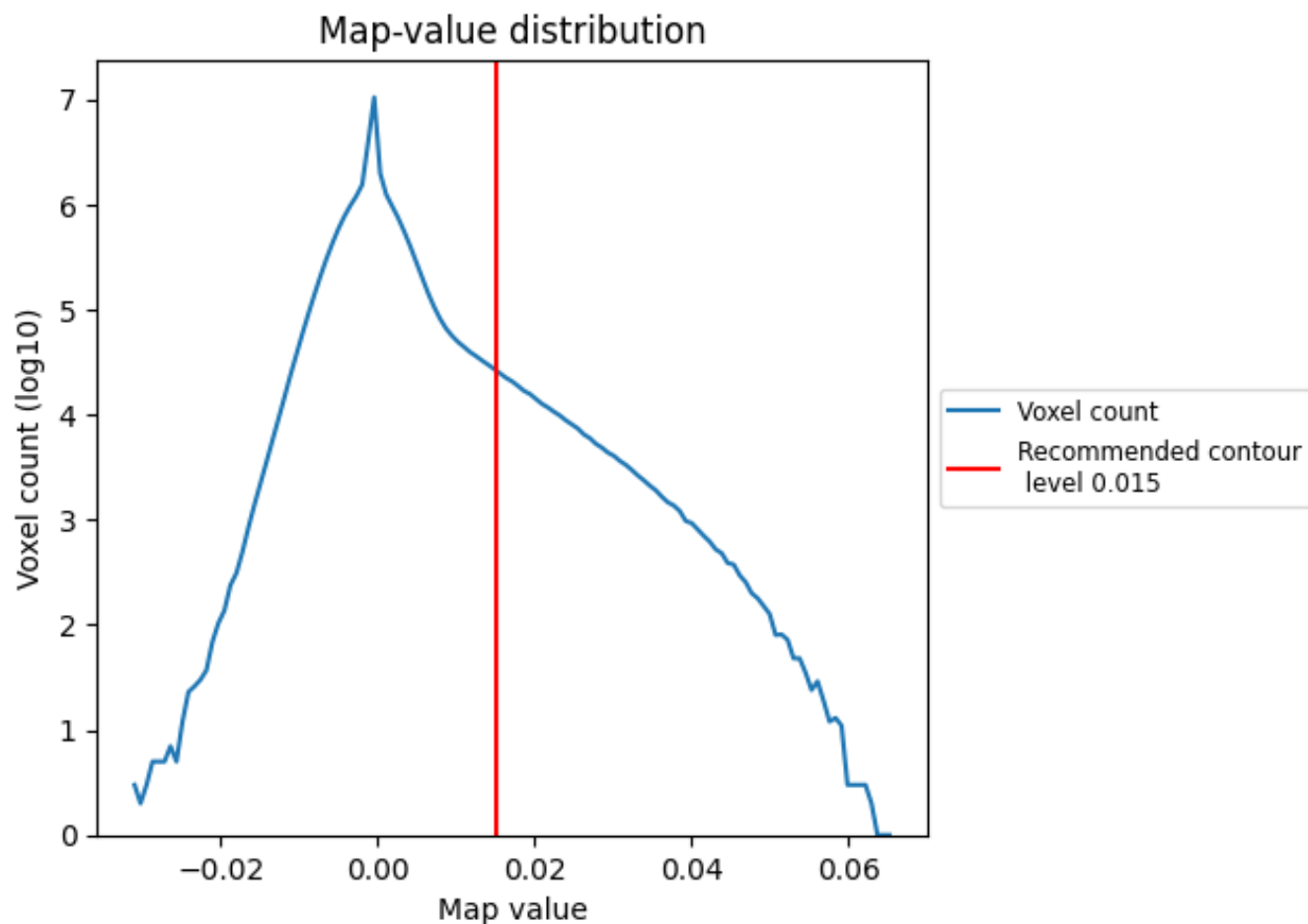
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

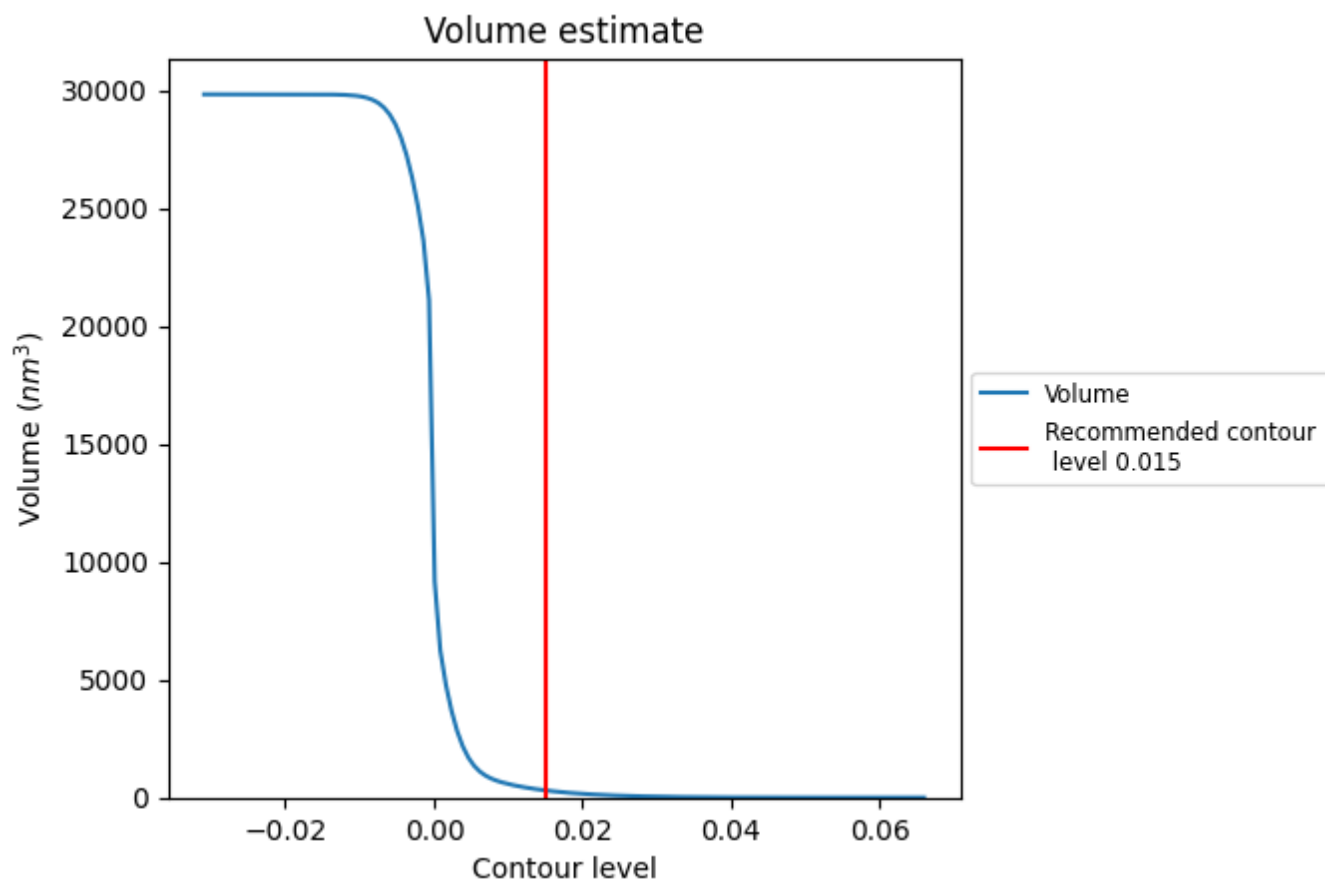
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

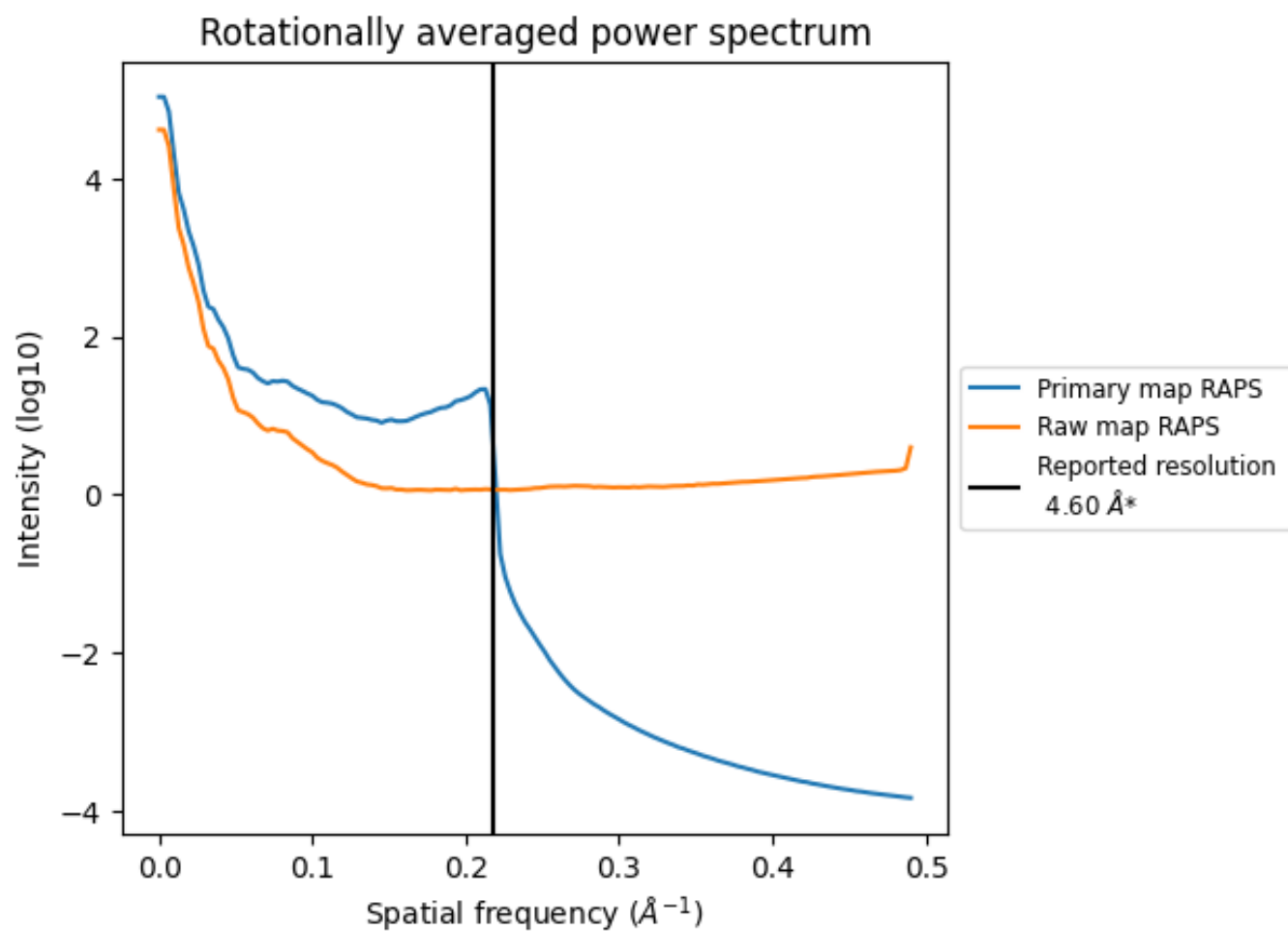
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

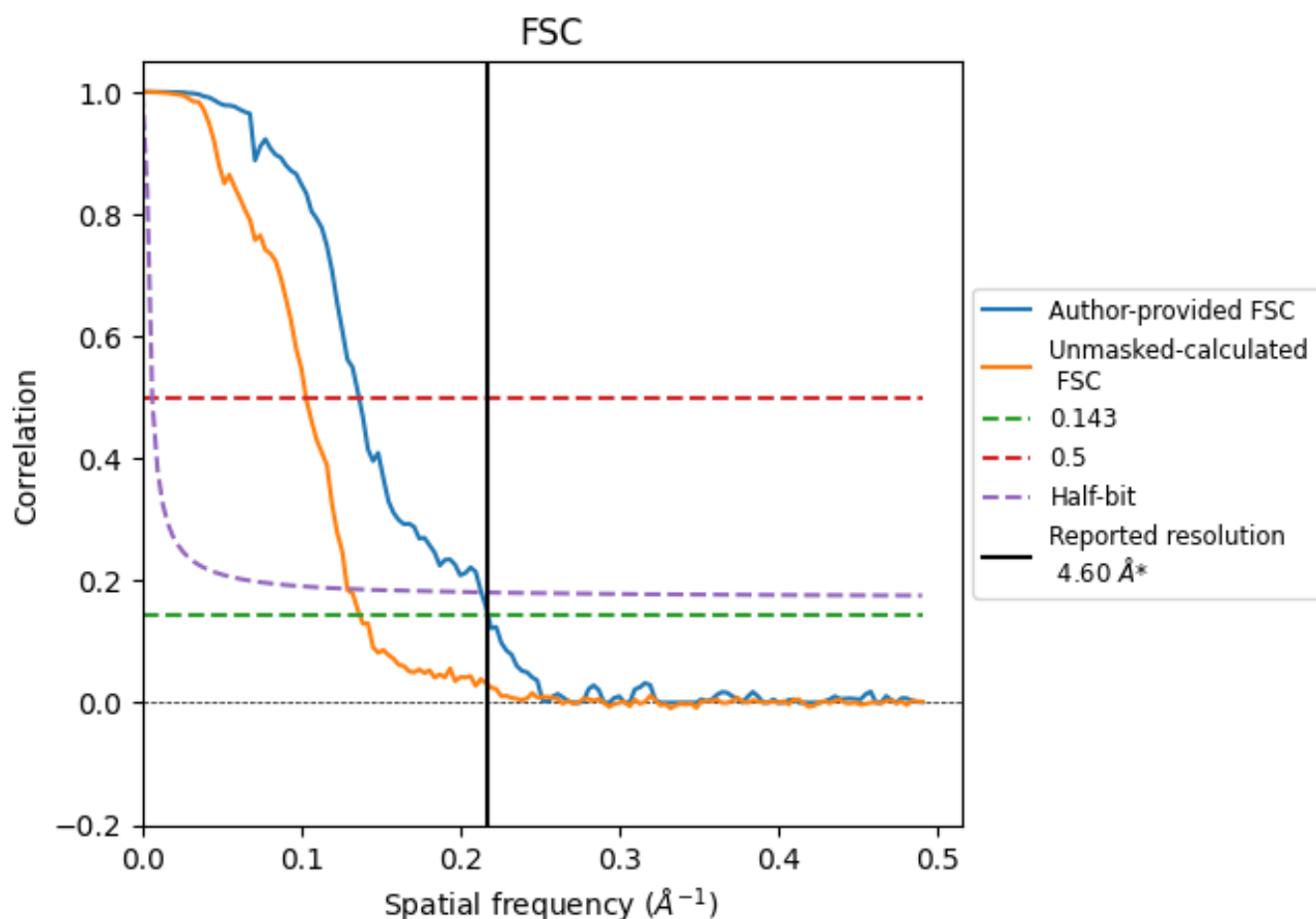


*Reported resolution corresponds to spatial frequency of $0.217 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

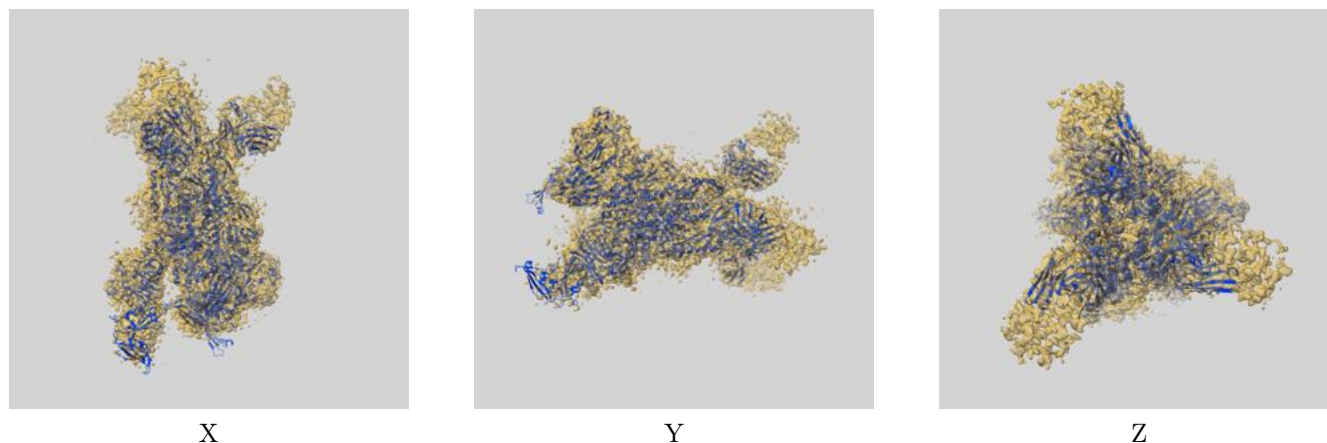
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.60	7.34	4.69
Unmasked-calculated*	7.31	9.72	7.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.31 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

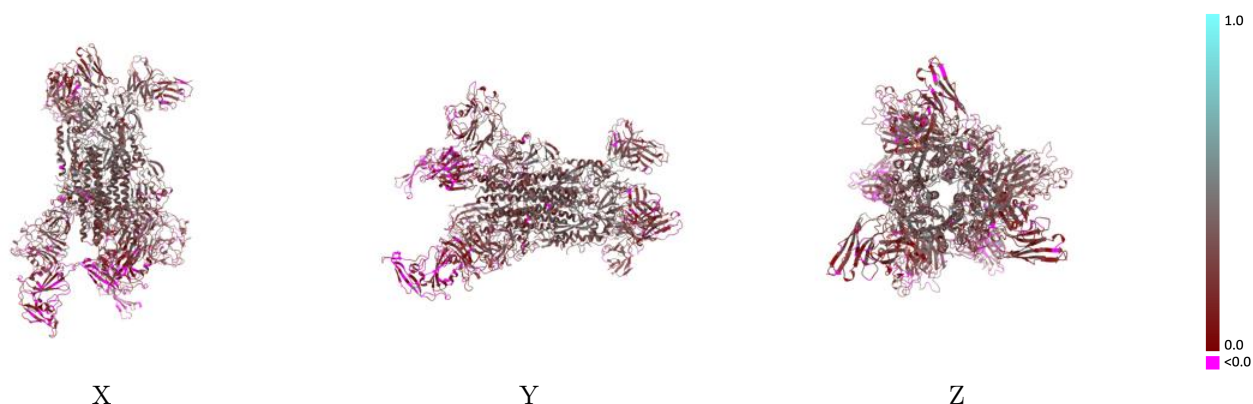
This section contains information regarding the fit between EMDB map EMD-8786 and PDB model 5W9K. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



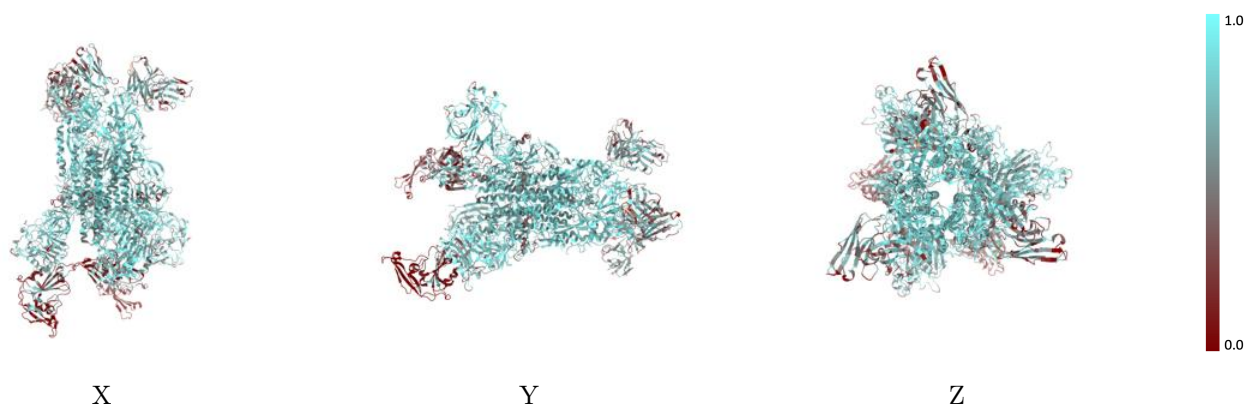
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



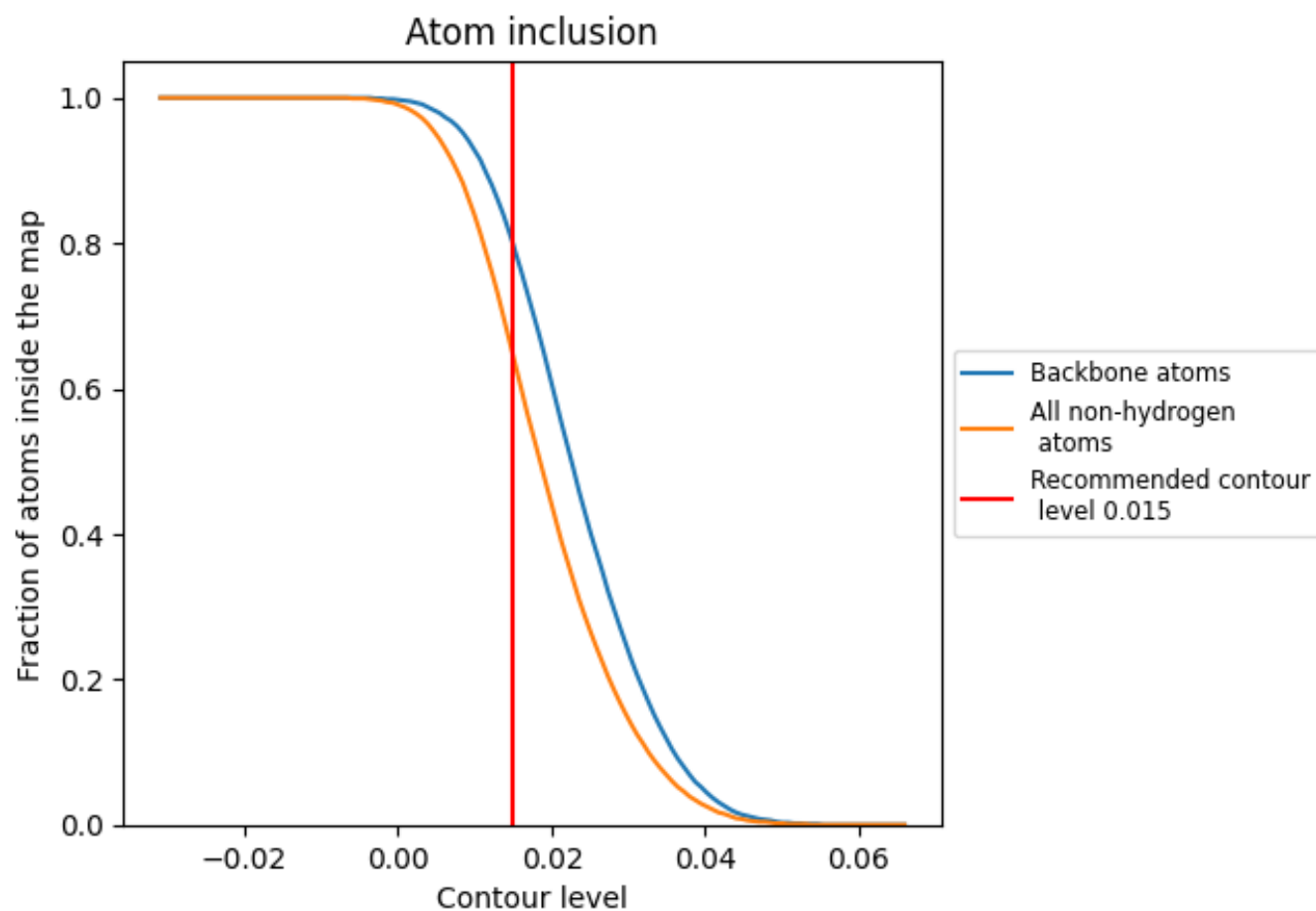
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6440	0.2420
A	0.7550	0.3120
B	0.5530	0.2290
C	0.4660	0.1920
D	0.7660	0.3240
E	0.5690	0.2430
F	0.4700	0.2050
G	0.7630	0.3280
H	0.5670	0.2480
I	0.4440	0.1870
J	0.5620	0.1840
K	0.6600	0.2120
L	0.6140	0.2020

